

University of Windsor

Scholarship at UWindor

Electronic Theses and Dissertations

Theses, Dissertations, and Major Papers

2011

Above Threshold Ionization and the Role of the Coulomb Potential

Atef Titi

University of Windsor

Follow this and additional works at: <https://scholar.uwindsor.ca/etd>

Recommended Citation

Titi, Atef, "Above Threshold Ionization and the Role of the Coulomb Potential" (2011). *Electronic Theses and Dissertations*. 474.

<https://scholar.uwindsor.ca/etd/474>

This online database contains the full-text of PhD dissertations and Masters' theses of University of Windsor students from 1954 forward. These documents are made available for personal study and research purposes only, in accordance with the Canadian Copyright Act and the Creative Commons license—CC BY-NC-ND (Attribution, Non-Commercial, No Derivative Works). Under this license, works must always be attributed to the copyright holder (original author), cannot be used for any commercial purposes, and may not be altered. Any other use would require the permission of the copyright holder. Students may inquire about withdrawing their dissertation and/or thesis from this database. For additional inquiries, please contact the repository administrator via email (scholarship@uwindsor.ca) or by telephone at 519-253-3000ext. 3208.

Above Threshold Ionization and the Role of the Coulomb Potential

by

Atef S. Titi

A Dissertation
Submitted to the Faculty of Graduate Studies
through the Department of Physics in Partial Fulfillment
of the Requirements for the Degree of Doctor of Philosophy at the
University of Windsor

Windsor, Ontario, Canada
2011

© 2011 Atef S. Titi

All Rights Reserved. No part of this document may be reproduced, stored or otherwise retained in a retrieval system or transmitted in any form, on any medium by any means without prior written permission of the author.

Above Threshold Ionization and the Role of the Coulomb Potential

by

Atef S. Titi

APPROVED BY:

WK. Liu, External Examiner
Department of Physics, University of Waterloo

G. WF. Drake, Advisor
Department of Physics

W.E. Baylis
Department of Physics

M. Schlesinger
Department of Physics

J. Gauld
Department of Chemistry and Biochemistry

S. Goodwin
Chair, Department of Computer Science

University of Windsor

10 May 2011

Author's Declaration of Originality

I hereby certify that I am the sole author of this thesis and that no part of this thesis has been published or submitted for publication.

I certify that, to the best of my knowledge, my thesis does not infringe upon anyone's copyright nor violate any proprietary rights and that the any ideas, techniques, quotations, or any other material from the work of other people included in my thesis, published or otherwise, are fully acknowledged in accordance with the standard referencing practices. Furthermore, to the extent that I have included copyright material that surpass the bounds of fair dealing within the meaning of the Canada Copyright Act, I certify that I have obtained a written permission from the copyright owner(s) to include such material(s) in my thesis and have included copies of such copyright clearances to my appendix.

I declare that this is a true copy of my thesis, including any final revisions, as approved by my thesis committee and the graduate studies office, and that this thesis has not been submitted for a higher degree to any other University or Institution.

Abstract

Within the single-active-electron approximation (SAE), an ab initio formulation of above threshold ionization (ATI) including rescattering that accounts for the long-range Coulomb potential is presented. From this ab initio formulation, an ad hoc formulation is developed in which the effect of the laser field is to split the atomic potential into two parts: a short range one responsible for rescattering producing the photoelectron high energy plateau, and a long-range Coulomb potential that affects the low energy electrons. Furthermore, the role of the Coulomb potential is investigated by looking at the low energy two dimensional momentum distributions, the momentum distributions along the polarization axis, and the low energy photoelectron energy spectra. Moreover, a formulation that considers the simultaneous transfer of both linear and angular momenta in the ionization process is developed. Finally, a formulation of high harmonic generation (HHG) is presented.

I dedicate this dissertation to my parents, my brothers' and sisters' and their families.

Acknowledgements

I would like to express my sincere gratitude and my deepest appreciation to my professor and advisor Dr. Gordon Drake for his invaluable advise, support, and his guidance. Without his help, suggestions, and availability throughout my research, this work could never have been finished. I will always strive and look up to him, to understand and appreciate physics the way he does.

I owe a special debt of thanks to Dr. William Baylis, and Dr. Mordechay Schlesinger, from the department of physics, for serving on my committee.

I am deeply grateful to Dr. Wing-Ki Liu, from the department of physics at the university of Waterloo, for serving on my dissertation as external examiner. Also, I am deeply grateful to Dr. James Gauld, from the department of chemistry and biochemistry, for agreeing- under a short time notice- to serve on my dissertation committee as external reader.

Special thanks are extended to Dr. Wladyslaw Kedzierski, the head of our department, for his support. Also, special thanks are extended to the faculty of graduate studies at the university of Windsor for their financial support during my studies.

I would be remiss if I did not acknowledge all the professors from whom I learned physics and mathematics. Dr. M.A. Ahmed, Dr. GI. Ghandour, Dr. D. Viggars, Dr. F. Majors, Dr. R. Khalil, Dr. B. Singh and Dr. M. A. Omar, all from Kuwait university. Dr. J.H. Macek, Dr. M. Quidry, Dr. T. Barnes, Dr. J. Burgdorfer, Dr. M. Brianing, Dr. E.

Harris, Dr. J. Cartwright, and Dr. D. Ferrel, all from the university of Tennessee. Dr.G. W.F. Drake (my advisor), Dr. E.H. Kim, and Dr. W.E. Baylis (for introducing Clifford algebra to me), all from the university of Windsor. For all of them, I am forever indebted.

Contents

Author's Declaration of Originality	iv
Abstract	v
Dedication	vi
Acknowledgements	vii
List of Figures	xii
1 Introduction	1
1.1 Basic concepts and terminology	1
1.2 Classical Considerations of Rescattering	4
1.3 Theoretical Methods	8
1.4 The Keldysh-Faisal-Reiss Theory-KFR	8
1.4.1 The Keldysh Approach	8
1.4.2 The Reiss Approach	10
1.5 The Present Work	12
1.5.1 The Final State Wave Function	13
1.5.2 Rescattering and Above Threshold Ionization	14
1.5.3 Rescattering And High Harmonic Generation	16
2 Theory I: Theoretical Background	18
2.1 Basic Elements of Time Dependent Formal Scattering Theory	18

2.1.1	The Green Functions	19
2.1.2	In and Out States	22
2.1.3	The S Matrix	24
2.2	S-Matrix Formalism with Two Potentials	27
2.3	The Volkov Wave Function	30
2.4	The Keldysh -Faisal- Reiss (KFR) Theory for Laser Induced Ionization: The Direct Electrons	32
2.4.1	Ionization by Circularly Polarized Electromagnetic Field	36
2.4.2	Ionization by Linearly Polarized Electromagnetic Field	38
3	Theory II	41
3.1	Difficulty in an <i>ab initio</i> Formulation of Rescattering	42
3.1.1	Regularization of Singularity	46
3.1.2	The Case of Circularly Polarized Electromagnetic Fields	56
3.1.3	The Case of Linearly Polarized Electromagnetic Fields	57
3.2	An <i>ad hoc</i> Formulation of Above Threshold Ionization	57
3.2.1	Evaluation of the Generalized Direct Term	60
3.2.2	Evaluation of the Rescattering Term	62
3.2.3	Rescattering Considerations with No Coulomb Effects	65
3.3	An <i>ab initio</i> Generalized <i>S</i> Matrix Formulation of Above Threshold Ionization	70
3.3.1	Evaluation of the Generalized <i>ab initio</i> Direct Term	72
3.3.2	Evaluation of the Generalized <i>ab initio</i> Rescattering Term	75
3.4	The Final State Wave Function	79
3.4.1	The Case of Circularly Polarized Light	86
3.4.2	The Case of Linearly Polarized Light	90
3.5	The Simultaneous Angular and Linear Momenta Considerations	93
3.5.1	Longitudinal Momentum Transfer in Multiphoton Ionization by Cir- cularly and Linearly Polarized Laser Fields	93
3.5.2	The Longitudinal Momentum Distribution	98
3.5.3	The ponderomotive Scattering Angle	105

3.6 High Harmonic Generation (HHG)	108
4 Numerical Results and Discussion	111
5 Conclusions	119
A Nordscieck Type Integrals	124
B Saddle-Point Method	128
C Numerical Integration Methods	132
C.1 Euler-Maclaurin Summation Formula	132
C.2 Fourier Transform Method	133
C.2.1 Computing Fourier Components	137
C.3 The Double Exponential Method	139
C.3.1 DE Formula For Oscillatory Integrals	141
C.3.2 DE Formula For Fourier Integrals	142
Bibliography	144
VITA AUCTORIS	149

List of Figures

- 3.1 Momentum distributions in the plane of polarization for strong field ionization of H(1s) from Martiny et al. [61]. Panels (a) and (b) show results obtained by solving the TDSE; panels (c) and (d) show results obtained using the Coulomb Volkov corrected SFA, while panels (e) and (f) show results obtained using SFA. The curves show $-\vec{A}(t)$, while the straight lines in (a) and (b) highlight the angular shift. The laser wavelength is 800 nm. . . . 81
- 3.2 Experimental distributions of parallel momentum (along polarization direction) for He atom in an intense 25 fs, 795 nm laser pulse at three peak intensities: $I = .6 \text{ PW/cm}^2$, $I = .8 \text{ PW/cm}^2$, $I = 1.0 \text{ PW/cm}^2$. The experimental data are taken from Rudenko et al. [74]. Notice the central minimum and the double peak structure. The SFA predicts a central maximum. . . . 82

3.3	<p>Experimental [(a), (c), and (e)] and calculated [(b), (d)] photoelectron spectra of Xenon from Quan et al. [79]. (a) $I = .08 \text{ PW/cm}^2$, $\lambda = 800, 1250, 1500,$ and 2000 nm from bottom to top, respectively. The complete spectra are shown in in the inset. The laser pulse durations are 40 fs at 800 nm, 30 fs at 1250 nm, and 1500 nm, while 90 fs at 2000 nm. (b) $I = .08 \text{ PW/cm}^2$ and $\lambda = 800, 1250, 1500,$ and 2000 nm, with Coulomb potential for the curves from bottom to top, respectively. While the uppermost curves is for $I = .08 \text{ PW/cm}^2$ and $\lambda = 2000 \text{ nm}$ without Coulomb potential. (c), (d) $\lambda = 2000 \text{ nm}$, $I = .032, .064 \text{ PW/cm}^2$ for the lower and upper curves respectively. (e) $\lambda = .04, .1 \text{ PW/cm}^2$ for the lower and upper curves respectively. In (c), and (e) the boundaries of the second hump are indicated by the dashed lines for higher intensities.</p>	83
3.4	<p>The measured Ne photoelectron distribution (crosses) is compared to the Rydberg refrence distribution (dots) and a reference Gaussian distribution centered at $p_z = 0$. The centre of the Ne distribution has a net $p_z > 0$. Courtesy of Smeenk et al. [82].</p>	103
3.5	<p>Net photoelectron longitudinal momentum p_z vs laser intensity calculated for linear and circularly polarized light. Courtesy of Smeenk et al. [82]. . . .</p>	104
4.1	<p>Differential ionization rates w_{fi}, in atomic units, of the hydrogen atom as a function of the kinetic energy of electron in units of U_p for $\theta_k = 0^\circ$. The cutoff at $10U_p$.</p>	112
4.2	<p>Differential ionization rates w_{fi}, in atomic units, of the hydrogen atom as a function of the kinetic energy of electron in units of U_p for $\theta_k = 10^\circ$. The cutoff at $9.6U_p$.</p>	113
4.3	<p>Differential ionization rates w_{fi}, in atomic units, of the hydrogen atom as a function of the kinetic energy of electron in units of U_p for $\theta_k = 20^\circ$. The cutoff at $9U_p$.</p>	114

4.4	Differential ionization rates w_{fi} , in atomic units, of the hydrogen atom as a function of the kinetic energy of electron in units of U_p for $\theta_k = 30^\circ$. The cutoff at $8U_p$	114
4.5	Differential ionization rates w_{fi} , in atomic units, of the hydrogen atom as a function of the kinetic energy of electron in units of U_p for $\theta_k = 40^\circ$. The cutoff at $6.6U_p$	115
4.6	Differential ionization rates w_{fi} , in atomic units, of the hydrogen atom as a function of the kinetic energy of electron in units of U_p for $\theta_k = 0^\circ$ red, 10° brown, 20° blue, 30° purple, and 40° green	115
4.7	Measured helium angle resolved photoelectron spectra for four different emission angles from Walker et al. [13]. The laser parameters are $I = 1.0 \text{ PW/cm}^2$, and $w = 1.58 \text{ eV}$. The polar plots show the measured angular distributions (crosses) at the indicated energies and the solid lines are only to guide the reader.	116
4.8	Calculated helium angle resolved photoelectron spectra for four different emission angles from Walker et al. [13] using semiclassical theory. The laser parameters are $I = 1.0 \text{ PW/cm}^2$, and $w = 1.58 \text{ eV}$	117
4.9	Differential ionization rates w_{fi} , in atomic units, of the hydrogen atom as a function of the kinetic energy of electron in units of U_p from Milošević et al. [59]. The calculations are in the length gauge. The lower curve includes rescattering with no Coulomb effects, while the upper curve includes both the Coulomb and rescattering effects. Both curves correspond to $\theta_k = 0^\circ$. The rounded tops (dotted lines) correspond to the angles $\theta_k = 20^\circ, 30^\circ$, and 40° and the cutoffs are at $9U_p, 8U_p$, and $6.6U_p$ respectively.	118

Chapter 1

Introduction

The field of intense-laser atom physics is broad and complex. The body of literature published in this field is extensive. In this chapter we will present basic concepts, terminology, and theoretical methods and models as well as literature pertaining to the work outlined in this dissertation. At the end of this chapter, we will outline the present work. Finally, an outline and organization of this dissertation is presented.

1.1 Basic concepts and terminology

With the discovery of above threshold ionization (ATI) by Agostini et al. (1979)[1] intense-laser atom physics entered the nonperturbative regime. These experiments recorded the photoelectron kinetic energy spectra generated by laser irradiation of atoms. Earlier experiments had measured total ionization rates by way of counting ions, and the data were well described by lowest-order perturbation theory (LOPT) with respect to the atom-field interaction [2], where the lowest order is the minimum number N of photons necessary for ionization. An ATI spectrum consists of a series of peaks separated by the photon energy and they indicate that an atom may absorb many more photons than the minimum number N required for ionization. Thus ATI is a highly nonlinear process. It is commonly accepted

by the atomic, molecular and optical (AMO) community to call the intensity domain of ATI the *multiphoton domain*.

When the energy spectrum of the ionized electrons appears to be a smooth, continuous spectrum, such a spectrum is taken by the AMO community to define what has come to be called the *tunneling domain*. To characterize the difference between *tunneling* and *multiphoton* ionization, Keldysh[3] introduced the so called adiabaticity parameter γ . Keldysh realized that the ionization process is very complex; it depends on three parameters—the radiation frequency ω , the electric field strength of radiation \mathbf{E} and the binding energy of the atomic electron E_i . According to his theory the rate of nonlinear ionization is determined by the adiabaticity parameter γ

$$\gamma = \omega(2E_i)^{\frac{1}{2}}/E \quad (1.1)$$

If $\gamma \gg 1$, the rate of nonlinear ionization w depends on the strength E as some power of E ,

$$w \sim \sigma^{(K)}(I/\omega)^K \quad (1.2)$$

Here $I = cE^2/8\pi$ is the intensity amplitude of the field, $\sigma^{(K)}$ is the generalized multiphoton cross section of the ionization process, which is like the one-photon cross section independent of the radiation intensity (depends on atomic structure, frequency and polarization of the radiation) and K is the *threshold number of absorbed photons*. Thus, in the limit $\gamma \gg 1$ the threshold process of nonlinear ionization is a multiphoton process.

If $\gamma \ll 1$, the rate of nonlinear ionization depends on the field strength E exponentially,

$$w \sim \exp\{-2(2E_i)^{\frac{3}{2}}/3E\} \quad (1.3)$$

which is the same as for tunneling ionization in a constant electric field [4].

The qualitative difference between multiphoton and tunnel ionization lies in the frequency dependence of the rates for these processes. According to (1.3) the dependence is zero for tunnel ionization, and significant for multiphoton ionization. According to (1.2) and (1.3) the threshold number K and also the generalized multiphoton cross section $\sigma^{(K)}$, which depends on the radiation frequency ω and atomic energy spectrum, determine this strong dependence.

Another feature of intense laser-atom interaction is what is called *high-order harmonic generation* (HHG). Atoms irradiated by intense lasers emit photon spectra which exhibit peaks at odd harmonics of the laser frequency. This was investigated experimentally by McPherson et al. (1987) [5] and Wildenauer (1987) [6]. The spectrum of this HHG displays a plateau (Ferry et.al. 1988) [7]; i.e., the initial decrease of the harmonic yield with increasing harmonic order is followed by a flat region where the harmonic intensity is more or less independent of its order. This plateau region terminates at some well defined order, the so-called cutoff.

Similarly, the experimental findings [8-15], reveal that the ATI process is more complex than has been assumed. These experiments and theoretical analysis [16-17] have shown new features of the ATI process, such as appearance of high energy plateaux that extend up to a cutoff energy around $10U_p$, where U_p is the ponderomotive energy, and the appearance of rings (sometimes called sidelobes) in the angular distribution of the ionized electrons.

As a consequence of the above experimental findings, Kulander et.al (1993) [18] and Corkum (1993)[19] introduced what is so called the *simple man model*. At some time t_0 , an electron enters the continuum due to ionization. Thereafter, the laser's linearly polarized electric field accelerates the electron away from the atomic core. However, when the electric field reverses direction, then, depending on the initial time of ionization t_0 , it may drive the electron back to the atomic core, where one of the following may happen:

- (1) The electron recombines into the ground state, emitting its entire energy—the sum of the kinetic energy that it acquired along its path plus the binding energy—in the form of one single photon. This beautifully explains the cutoff energy of the plateau of the HHG, as well as the fact that the yield of HHG strongly decreases when the laser field is elliptically polarized. In this case the electron misses the ion.
- (2) The electron may scatter inelastically off the atomic core. In particular, it may knock off a second electron from the atomic core. This is what is called *nonsequential double ionization*
- (3) The electron may scatter elastically off the atomic core, where, it can acquire drift energies much higher than otherwise, thus contributing to the extended high energy plateau

of the ATI.

1.2 Classical Considerations of Rescattering

Classically, an electron promoted at time t_0 into the continuum due to ionization, will start its trajectory with zero velocity at the classical exit of the tunnel, which, for strong fields, is a few atomic units away from the position of the atomic core. This small offset is ignored and we will have the electron's trajectory start at $\vec{r}(t = t_0) = 0$, which is the position of the ion with $\vec{v}(t = t_0) = 0$ (although quantum mechanically, this violates Hiesenberg uncertainty principle, it produces no significant error for linearly polarized fields; however, for circularly polarized field, caution should taken regarding the above assumption due to quantum mechanical considerations of angular momentum). Next, ignoring the influence of the atomic core, the electron trajectory will evolve in the strong laser field according to the classical equations of motion and hence its velocity is

$$m\vec{v}(t) = e(\vec{A}(t_0) - \vec{A}(t)) \equiv \vec{P} - e\vec{A}(t), \quad (1.4)$$

Where e is the electron charge and $\vec{A}(t)$ is the vector potential. The first term $\vec{P} \equiv e\vec{A}(t_0)$ is constant, which is the drift momentum measured at the detector and the second term oscillates in phase with the vector potential $\vec{A}(t)$. The time averaged kinetic energy of this electron, over one period T is

$$E = \frac{m}{2} \langle \vec{v}(t)^2 \rangle_T = \frac{\vec{P}^2}{2m} + \frac{e^2}{2m} \langle \vec{A}(t)^2 \rangle_T \equiv E_{\text{drift}} + U_P \quad (1.5)$$

Where $\vec{A}(t)$ is chosen such that $\langle \vec{A}(t) \rangle_T$ is zero and U_P is the ponderomotive energy

$$U_P = \frac{e^2}{2m} \langle \vec{A}(t)^2 \rangle_T, \quad (1.6)$$

is the cycle-averaged kinetic energy of the electron's wiggling motion. Of course if $\vec{v}_0 \neq 0$ at t_0 , then $e\vec{A}(t_0)$ in (1.4) has to be replaced by $e\vec{A}(t_0) + m\vec{v}_0 \equiv \vec{P}$.

For a general elliptically polarized laser field, with ellipticity η , the vector potential $\vec{A}(t)$ is

$$\vec{A}(t) = \frac{A}{\sqrt{1 + \eta^2}} (\hat{i} \cos(\omega t) + \eta \hat{j} \sin(\omega t)) \quad (1.7)$$

and ponderomotive energy $U_P = \frac{(eA)^2}{4m}$. The drift energy $E_{\text{drift}} = \frac{(e\mathbf{A}(t_0))^2}{2m}$ is restricted to the interval

$$\frac{2\eta^2}{1+\eta^2}U_P \leq E_{\text{drift}} \leq \frac{2}{1+\eta^2}U_P \quad (1.8)$$

For linear polarization ($\eta = 0$), it can acquire any value between 0 and $2U_P$, whereas for circular polarization ($\eta = 1$) it is restricted to the value U_P . As we shall see later (see Chapter 3); quantum mechanics softens these bounds, however, they are useful as signature in the analysis of experimental spectra (Bucksbaum et.al., 1986 and 1988)[20-21] in particular for high intensity (Mohideen et.al., 1993; Reiss, 1996)[22;23]

We may recall that the ionization probability depends on the electric field, while the drift momentum $\vec{P} = e\vec{A}(t_0)$ is proportional to the vector potential, both at time t_0 of ionization. The probability of a certain drift momentum is weighted with the ionization rate at time t_0 . The electron is mostly ionized when the magnitude of the electric field is near its maximum. Then, for linear polarization, the vector potential and hence the drift momentum are near zero. To reach a maximal drift energy of $2U_P$, the electron must be ionized when the electric field is near zero, and hence the ionization rate is very low. This is consistent with the low energy part of the ATI spectrum, where a pronounced drop of ionization rates with increasing energy occurs.

As a consequence of the evolution of the electron trajectory in the strong laser field, the electron may return back to the atomic core and rescatter. We can integrate the electron velocity (1.4) to obtain its trajectory

$$\vec{r}(t) = \frac{e}{m} \left((t - t_0)\vec{A}(t_0) - \int_{t_0}^t d\tau \vec{A}(\tau) \right) \quad (1.9)$$

For the electron to return to the atomic core at some time $t_1 > t_0$, then $\vec{r}(t_1) = 0$. For linear polarization along the z - axis, this implies $z(t_1) = 0$, and $x(t) \equiv y(t) \equiv 0$. This gives the time of return t_1 as a function of the ionization time t_0 . To this end, the kinetic energy of the electron at the time of return, as given by (1.4) is

$$E_{\text{ret}} = \frac{e^2}{2m} [A(t_1) - A(t_0)]^2. \quad (1.10)$$

Maximizing this energy with respect to t_0 under the constraint that $z(t_1) = 0$ yields $E_{\text{ret}}^{\text{max}} = 3.17U_P$ for $wt_0 = 108^\circ$ and $wt_1 = 342^\circ$ (Corkum, 1993; Kulander et.al., 1993)[19;18]. If at the moment of return the electron recombines with the ion into the ground state, emitting its kinetic energy plus the the ionization energy in the form of one photon of frequency w' , then the maximum energy of the emitted photon will be given by

$$\hbar w'_{\text{max}} = |E_i| + 3.17U_P \quad (1.11)$$

where $|E_i|$ is the ground state ionization energy. This is precisely the cutoff law for HHG.

Instead of recombining and emitting a harmonic photon, the ionized electron can rescatter elastically at the moment of return t_1 thereby attaining much higher energy (quantum mechanically the electron will pick up further electrons due to continuum-continuum transitions). To see this, suppose that at $t = t_1$ the electron back scatters by 180° , so that $mv_z(t_1^-) = e[A(t_0) - A(t_1)]$ just before and $mv_z(t_1^+) = -e[A(t_0) - A(t_1)]$ just after backscattering. Then for $t > t_1$, the electron velocity is again given by (1.4) but we have to add to it the electron velocity $mv_z(t^+)$ and therefore

$$\begin{aligned} mv_z(t) &= e(A(t_1) - A(t)) - e[A(t_0) - A(t_1)] \\ mv_z(t) &= e(2A(t_1) - A(t_0)) - eA(t) \end{aligned} \quad (1.12)$$

For a laser pulse of duration τ_0 , then for $t \gg \tau_0$, $A(t) = 0$ and therefore $mv_z(t) \equiv P_z = e[2A(t_1) - A(t_0)]$ so that

$$E_{\text{bscat}} = \frac{e^2}{2m} [2A(t_1) - A(t_0)]^2 \quad (1.13)$$

This is the energy of the backscattered electron registered at the detector ($t \gg \tau_0$). Maximizing E_{bscat} under the constraint $z(t_1) = 0$ yields $E_{\text{bscat}}^{\text{max}} = 10.007U_P$ (Paulus et al., 1994) [24] for $wt_0 = 105^\circ$ and $wt_1 = 354^\circ$. The rescattering plateau in the energy spectrum with its cutoff at $10U_P$ was identified by Paulus et al. (1994) [10,11]. Indeed, the experimental measurement of Walker et al., (1996) [13] and Sheehy et.al., (1998) [15] for He at intensities around 10^{15} W/cm^2 show an extended plateau for energies between $2U_P$ and $10U_P$.

If we consider rescattering into an arbitrary angle θ_0 with respect to the electron's initial direction upon its return to the ion, then its momentum just before rescattering is

$P_z = e(A(t_0) - A(t_1))$. However, just after rescattering the magnitude of the momentum is still $|A(t_0) - A(t_1)|$ but with two components P_z and say, P_y . Then for times $t \gg t_1$ we have

$$P_z(t) = e[A(t_1) - A(t)] - e \cos(\theta_0)|A(t_0) - A(t_1)|, \quad (1.14)$$

$$P_y(t) = e \sin(\theta_0)|A(t_0) - A(t_1)| \quad (1.15)$$

Of course when the electron leaves the laser pulse, an electron that was scattered by the angle θ_0 arrives at the detector at an angle θ (with respect to the direction of linear polarization) given by

$$\frac{\langle P_z(t) \rangle_T}{\langle P_y(t) \rangle_T} = \cot(\theta) = \cot(\theta_0) - \frac{A(t_1)}{\sin(\theta_0)|A(t_0) - A(t_1)|} \quad (1.16)$$

Again, for $t \gg \tau_0$, the kinetic energy at the detector (outside the pulse) is

$$E_{\text{kin}} = \frac{e^2}{2m} \{A(t_0)^2 + 2A(t_1)[A(t_1) - A(t_0)](1 \pm \cos(\theta_0))\} \quad (1.17)$$

The kinetics contained in (1.16) and (1.17) indicates that for rescattering into an arbitrary angle θ with respect to the direction of linearly polarized laser field, we expect a lower maximal energy since part of the maximal return energy $3.17U_P$ of the returning electron will go into the transverse motion. This implies, for fixed energy E_{kin} there is a cutoff in the angular distribution; that is to say, rescattering will only be recorded for angles such that $0 \leq \theta \leq \theta_{\text{max}}(E_{\text{kin}})$. These are what are called sidelobes (or rings) in the angular distribution of the ejected electrons as were first observed by Yang et al. (1993) [9].

Besides its simplicity, the *simple man model*, introduces the concept of *rescattering* in intense laser-atom physics, where ionized electrons may be driven back by the laser's electric field to the atomic core and rescatter. Pre-existing theories, the so called Keldysh-Faisal-Reiss (KFR) theory [3,25-27] or also called the *strong-field approximation* (SFA) [28-29] account for direct electrons only. These electrons, after the ionization process, never interact with the atomic core. Instead they simply leave the laser field and are observed experimentally. Thus a quantum mechanical treatment of rescattering is needed to improve existing theories in order to explain the above mentioned features. Such early attempts were embedded in fully quantum mechanical descriptions of HHG (Lewenstein et al., 1994; Becker et al., 1994) [30;31] and ATI (Becker et al., 1994; Lewenstein et al., 1995) [32;33].

1.3 Theoretical Methods

The *single-active-electron approximation* (SAE) replaces the atom in the laser field by a single electron that interacts with the laser field and is bound by an effective potential so optimized as to reproduce the ground state and singly excited states. While multiple electrons may be ionized, multielectron effects appear to be absent from above threshold ionization of photoelectron spectra. Comparison of experimental ATI spectra in argon with spectra calculated numerically by Nandor et al. (1999) [16] confirms the validity of the SAE.

The main theoretical approaches can be divided into two groups. The first [34-41] is rather complicated, requiring a large amount of computation time either for Floquet calculations or direct integration of the time dependent Schrödinger equation. The second has its origin in the KFR theory of ionization in strong electromagnetic fields which was formulated by Keldysh [3] in 1964 and later both Faisal (1973) [25] and Reiss (1980) [26] presented modifications of this theory which is now known also as the *strong field approximation* (SFA) [28,29].

1.4 The Keldysh-Faisal-Reiss Theory-KFR

Essentially, the KFR theory is determined by the zeroth order term of an expansion of the S-matrix in terms of the atomic potential V_c while the interaction with the laser field is implicitly taken care to all orders by the Gordon-Volkov wave function that describes the outgoing electron in the laser field [42]. The theoretical formulation of this work is based on the KFR theory.

1.4.1 The Keldysh Approach

In his pioneering work for the detachment of an electron from a short-range potential Keldysh [3], started from the exact expression for the transition amplitude from an initial bound state i to a final state f in the continuum which is given by the scattering S matrix

element (Details are presented in Chapter 2 of this work)

$$S_{\text{fi}}(t) = -i \int_0^t \langle \Psi_{\text{f}} | V(r, t') | \Psi_{\text{i}}^0 \rangle dt' \quad (1.18)$$

Here $\Psi_{\text{i}}^0(r, t')$ is the unperturbed wave function of the initial bound state i ; $\Psi_{\text{f}}(r, t')$ is the exact wave function of the final state with fixed momentum \vec{P} , taking into account the interaction potential $V(\vec{r}, t')$ of the electron with the electromagnetic field.

The exact wave function cannot be written analytically. The *Keldysh approximation* [3] consists of the replacement of Ψ_{f} by the wave function $\Psi_{\text{f}}^{\text{v}}$ of a free electron in an external electromagnetic field. This approximation is correct if in the final state the effect of atomic potential on the ejected electron can be neglected. This holds, partially, for the case of a short-range potential (for example, the detachment of negative ions).

In his original formulation Keldysh used what is commonly called the *length gauge* for the interaction of an electron with an electromagnetic field in the dipole approximation

$$V(r, t) = e \vec{r} \cdot \vec{E} \quad (1.19)$$

Here \vec{E} is the electric field of the radiation wave and \vec{r} is the electron coordinate. The wave function Ψ^{v} of the final state with momentum \vec{P} is

$$|\Psi^{\text{v}}\rangle = |\vec{P} + e\vec{A}/c\rangle e^{-iS(\vec{p}, t)} \quad (1.20)$$

Where $|\vec{P} + e\vec{A}/c\rangle$ is a plane wave, $S(\vec{p}, t)$ is the semiclassical action for an electron in the electromagnetic field and $\vec{A}(t)$ is the vector potential of the field related to the electric field \vec{E} by $\vec{E}(t) = -(1/c)d\vec{A}(t)/dt$. The above wave function is the *Volkov* wave function in the *length gauge*. [42]

For the case of a linearly polarized field and using the saddle-point method (see Appendix B) to calculate the integral over time, Keldysh obtained the following simple expression for the ionization rate $w = S_{\text{fi}}(t)^2/t$

$$w \sim \exp\{-(2E_{\text{i}}/\omega)[(1 + 1/2\gamma^2) \sinh^{-1} \gamma - (1/2\gamma)(1 + \gamma^2)^{\frac{1}{2}}]\} \quad (1.21)$$

Where E_{i} is the initial bound state energy, ω is the radiation frequency and Keldysh adiabaticity parameter γ which is given by (1.1). In the limiting cases $\gamma \gg 1$ and $\gamma \ll 1$

for the adiabaticity parameter γ we obtain from (1.7) the multiphoton limit (1.2) and the tunneling limit (1.3), respectively. It is to be emphasized that Keldysh original approach is a threshold ionization one (it does not account for above threshold ionization). However, Keldysh original approach provides us with the physical understanding of the concept of tunneling.

The Keldysh parameter γ can be defined by the ratio $\gamma = \tau/T$. Here τ is the time required by the atomic electron to tunnel through the potential barrier, formed at a certain moment of time t by the sum of the atomic Coulomb potential $V_c(\vec{r})$ and the electric dipole potential of the laser field $V(\vec{r}, t)$ as given by (1.5), whereas $T = 2\pi/\omega$ is the period of the radiation field oscillations. If $\gamma \ll 1$, then the ionization takes place quasi-instantaneously by tunneling of the electron through the barrier at a particular instant of time, whereas for $\gamma \gg 1$ the laser field performs during ionization many oscillations and therefore multiphoton ionization prevails. A more suitable definition of the Keldysh parameter is to consider the expression $\gamma = \tau\omega$. An electron born by tunneling will exit at a distance r determined by $|E_i| = e r E$. The tunneling time τ is determined through the exit distance r and the tunnel velocity v_τ , namely $r = v_\tau \tau$. On the other hand we can assume that, since the electron initially in the ground state, the tunnel velocity v_τ is equal to electron velocity on the first Bohr orbit $v_\tau = v_0 = \alpha c$, where $\alpha = e^2/\hbar c$ is the fine structure constant, then we find from the foregoing two relations $\tau = r/v_\tau = |E_i|/e E \alpha c$ and consequently the Keldysh parameter can be expressed as,

$$\gamma = \tau\omega = \sqrt{\frac{|E_i|}{2U_p}} \quad (1.22)$$

where U_P is the ponderomotive potential which is defined as the average kinetic energy of the electron in the laser field. Of course equations (1.1) and (1.22) are equivalent.

1.4.2 The Reiss Approach

Reiss [26] used another gauge of the interaction between an electron and an electromagnetic field, the so called *velocity gauge*

$$V(\vec{r}, t) = \frac{e}{mc} \vec{P} \cdot \vec{A}(t) + \frac{e^2}{2mc^2} \vec{A}(t)^2 \quad (1.23)$$

Here \vec{P} is the quantum mechanical operator of the electron momentum. In this case the wave function of the final continuum state takes a form different from (1.20):

$$|\Psi_f^y\rangle = |\vec{P}\rangle e^{-iS(\vec{p},t)} \quad (1.24)$$

Again, $|\vec{P}\rangle$ is a plane wave and $S(\vec{P},t)$ is the semiclassical action of an electron in a magnetic field. This wave function is called the *Volkov wave function* in the *velocity gauge*.

The Keldysh approximation is not *gauge invariant*; therefore the Keldysh and Reiss approaches result in different values of ionization rate.

The simplest results are obtained with the Reiss approach [27]. For a circularly polarized field, the ionization rate with the ejection of an electron into a solid angle $d\Omega$ (details are in Ch.2),

$$dw/d\Omega \sim \sum_{S=0} (E_i + P_{K+S}^2) P_{K+S} |\Psi_i^{(0)}(P_{K+S})|^2 \cdot J_{K+S}^2(2U_P P_{K+S} \sin(\theta)) \quad (1.25)$$

Here $K+S$ is the number of absorbed photons, P_{K+S} is the electron momentum in the final state, so that according to the energy conservation law, for absorption of $K+S$ photons we have

$$\frac{1}{2} P_{K+S}^2 = (K+S)w - U_P - E_i \quad (1.26)$$

Again, here E_i is the binding energy of the ground state, $\Psi_i^{(0)}(P_{K+S})$ is the the initial wave function in the momentum representation and J_{K+S} is the Bessel function and θ is the angle between the vector \vec{P}_{K+S} and the direction of propagation of the circularly polarized field. It is easy to see that most electrons are ejected in the polarization plane of the field when $\theta = \pi/2$.

The sum in (1.25) begins with the threshold value $K(S=0)$ so that the first $P_K^2 > 0$. The next term determines the absorption of the so called above threshold photons, and S is the number of such photons. So unlike the Keldysh approach which is a threshold ionization theory, Reiss approach is an above threshold ionization theory. Another advantage of the Reiss method over the Keldysh method is that it is not necessary that the ionization be multiphoton, unlike the case of the Keldysh method. In particular, (1.25) gives the correct result for one-photon ionization when this process is allowed by the energy conservation

law (1.26). This is because Keldysh used the saddle-point method in the calculation of the ionization rate. No such approximation is used in Reiss approach. This is the advantage of the *velocity gauge*.

Faisal [25] developed an approach similar to the Keldysh approximation. However, in the amplitude given in (1.18) the final state was taken to be unperturbed by the external laser field while the initial bound state does take into account this perturbation. Reiss [28] has shown that the Faisal approach is essentially the same as the Keldysh approach.

The Keldysh-Faisal-Reiss (KFR) theory is also called the strong field approximation (SFA) [28,29]. The essence of this approximation, as emphasized by Reiss [43], consists of the following:

- (1) The use of the time reserved form of the S matrix.
- (2) the use of the velocity gauge.
- (3) When $2U_P/E_i \gg 1$, replace the final wave function in (1.18) by the Volkov wave function.

The physical picture of tunneling associated with the length gauge has no analog in the velocity gauge. The SFA only demands condition (3) to be satisfied.

1.5 The Present Work

It is quite clear from the preceding discussion that it is necessary to improve the existing theory by:

- (1) Improving the final wave function to take into account the long range nature of the Coulomb potential. This will modify the ionization rates, but will not account for rescattering.
- (2) going to the next term in the S-matrix expansion to include rescattering to account for the high energy plateau of the ATI and HHG.

Due to the association of the physical picture of tunneling with the length gauge, most of the AMO community prefer the length gauge and the majority of publications utilize the length gauge. In this work we share the belief of Reiss [43]; Delone [44] that the theory based on the velocity gauge is capable of accounting for ATI and HHG. Our theoretical

formulation is carried in the velocity gauge.

1.5.1 The Final State Wave Function

In order to improve the KFR theory for ATI, Trombetta et al. [45] and Basille et al. [46], suggested to use for the final continuum state of the electron, the Coulomb-Volkov wave function $\Psi_{\vec{k}}^{(cv)}$, introduced earlier by Jain and Tzoar [47]

$$|\Psi_{\vec{k}}^{(cv)}\rangle = \exp\{-iS(\vec{k}, t)\} e^{\pi a/2} \Gamma(1 + ia) |\vec{k}\rangle {}_1F_1[-ia, 1, -i(kr + \vec{k} \cdot \vec{r})] \quad (1.27)$$

Where $a = Z/k$. Mittleman (1994) obtained the same wave function variationally [48]. If we set $a = 0$ we recover the Volkov wave function.

Later, an improved version of the Coulomb-Volkov wave function was suggested by Kamiński et al. [49-56], and Milosovic et al. [57-59], which is called the improved Coulomb-Volkov state ansatz,

$$\begin{aligned} |\Psi_{\vec{Q}}^{(icv)}\rangle &= \exp\{-iS(\vec{k}, t)\} e^{\pi a/2} \Gamma(1 + ia) |\vec{k}\rangle {}_1F_1[-ia, 1, -i(Qr + \vec{Q} \cdot \vec{r})] \quad (1.28) \\ \vec{Q} &= \vec{k} + \frac{e}{c} \vec{A} \end{aligned}$$

These new improved wave functions are suitable for linearly polarized laser fields. In a recent experiment by Eckle et al. (2009) [60], published in the journal Science, the photoelectron momentum distributions show counter-intuitive shifts. They irradiated He with a circularly polarized femtosecond pulse with parameters suitable for the tunneling regime and invoked the concept of tunneling time to explain the shift. Aware of the experiment, Martiny et al. [61] solved the three dimensional Schrödinger equation for a short circularly polarized pulse interacting with an H atom. The photoelectron momentum distributions show counter intuitive shifts, similar to those observed by Eckle et al. [60]. Furthermore the Martiny et al. [61] calculation shows these shifts in the multiphoton regime. They explained the shifts in terms of angular momentum considerations. The shifts are a manifestation of the fact $\langle \Psi | L_z | \Psi \rangle = \langle L_z \rangle \neq 0$ after the pulse, which implies that the azimuthal velocity is nonvanishing, which in turn, makes the distribution rotate compared to the $\langle L_z \rangle = 0$ case. The H atom is initially in the ground state and hence, $\langle L_z \rangle = 0$, before the pulse.

According to Ehrenfest's theorem,

$$\frac{d}{dt} \langle L_z \rangle = i \langle [H, L_z] \rangle \quad (1.29)$$

which forces the liberated electron to pick up a nonzero value of $\langle L_z \rangle$, since $[H, L_z] \neq 0$ during the pulse for $H = H_o + \vec{A} \cdot \vec{P} + \frac{A^2}{2}$, H_o being the free Hamiltonian. The mean value of L_z changes during the pulse, in accordance with Ehrenfest's theorem, until it becomes a constant with the value

$$\langle L_z \rangle = i \int_0^T \langle [H, L_z] \rangle dt \quad (1.30)$$

after the pulse. Although $[H, L_z] \neq 0$, it remains true that, $\langle [H, L_z] \rangle = 0$ for Volkov state. Moreover, their calculations using the Coulomb-Volkov wave function show little or no shift. This doesn't represent a problem for the case of linear polarization, since there is no net transfer of angular momentum during ionization. However this is not the case for circular polarization, since there is N units of angular momenta transferred during ionization, where N is the number of absorbed photons. Martiny et al. [61] suggest that an improved wave function that is suitable for circular polarization will produce such shifts. *In this work we introduce such a wave function*, and show that the above considerations are taken into account.

1.5.2 Rescattering and Above Threshold Ionization

It will be shown in Ch. 3, that the S-matrix for the transition from initial bound state i to a final continuum state f is given by,

$$\begin{aligned} (S - 1)_{fi} &= -i \int_{-\infty}^{\infty} dt \langle \Psi_f^{(-)}(t) | V_{\text{int}}(t) | \phi_i(t) \rangle \\ &\quad -i \int_{-\infty}^{\infty} dt \int_{-\infty}^t dt' \int d\vec{q} \langle \Psi_f^{(-)}(t) | V_s | \Psi_{\vec{q}}(t) \rangle \langle \Psi_{\vec{q}}(t') | V_{\text{int}}(t') | \phi_i(t') \rangle \end{aligned} \quad (1.31)$$

The physical meaning of (1.31) is as follows. Due to the interaction with the laser field, the electron gets ionized from the initial ground state. After that, the electron propagates

in the laser field and it also feels the long-range Coulomb field. It can then leave these fields and be observed experimentally, and this corresponds to the first term of the right hand side of (1.31). It can, however, happen that during this propagation the ionized electron comes back to the atomic core and scatters at the short range of the atomic potential. After rescattering, the electron propagates out of these fields and can be observed. Of course, both contributions interfere quantum mechanically as shown in (1.31)

The difficulty in (1.31) comes from the second term. Its an eleven-fold integral. Exact numerical evaluation of the amplitude (1.31) for a finite range binding potential is very cumbersome. The temporal integrals are highly oscillatory and extend over the infinite half plane. The integration over the intermediate continuum states $\Psi_{\vec{q}}$ can be done analytically using the saddle-point approximation (Lewestein et al. [30], Lewestein et al. [33], Milosevic et al. [58], Milosevic et al. [59]). For a zero-range potential, however, the spatial integration in the matrix elements becomes trivial, and if we expand the intermediate and the final continuum states in terms of Bessel functions, then the temporal integration over the time t can be carried out analytically and yields a Dirac delta function. The remaining integration over t' has to be carried out numerically, as was done by Lohr et al. [62] and Milosevic et al. [58] for linearly polarized fields. Alternatively, the integral over t' may be done first numerically, and the integral over t can then be evaluated using fast fourier transform method (Milosevic [59]). It is to be mentioned that Milosevic [58,59] and Lohr [62] used the length gauge and only Milosevic [59] considered rescattering with Coulomb effects.

Attempts to evaluate (1.31) in the velocity gauge for atomic short range potentials were carried by Bao et al. (1996) [63] and Usachenko et al. (2004) [64]. Both considered rescattering with no Coulomb effects. Bao et al. [63] expanded the intermediate and final Volkov states in terms of Bessel functions and generalized Bessel functions [26] then both the temporal integrals over t and t' were carried out analytically. The remaining integral over \vec{q} was carried out numerically. Usachenko et al. [64] did the same for both temporal integrals; however, for the integral over \vec{q} , he employed the method of essential states (the pole approximation) [65,66]. States are called essential if they are populated during the entire process of ATI. Basis states of the Hamiltonian are restricted to only the essential

states. These are continuum states which differ from each other by the energy of one photon of the laser field. The drawback of the approach of Bao et al. and Usachenko et al is that in addition they end up with double sums of products of generalized Bessel functions, and these generalized Bessel functions are difficult to evaluate numerically, especially if the order of photons absorbed in ATI is high.

In this work we will evaluate (1.31), in the velocity gauge, numerically. First, we will consider rescattering without coulomb effects and second we will consider rescattering with Coulomb effects. *To our best knowledge no such calculations have ever been done.* In both cases we will employ a recently introduced powerful numerical quadrature for the accurate evaluation of slowly decaying highly oscillatory functions that extend over the infinite half plane [67-68]. To our best knowledge, we will be the first to introduce this method to the AMO community. We will evaluate the integral over t' first using this method and then using the fast fourier transform method to evaluate the integral over t . By then, we are at a position to test our theoretical formulation against the experimental results of [13,15].

1.5.3 Rescattering And High Harmonic Generation

In our theoretical formulation for the description HHG, the wave function $|\Psi(t)\rangle$ will have a ground state $|\phi_i\rangle$ component, to allow recombination, and continuum components $F(\vec{q}, t)$. Therefore, the dipole matrix element

$$X(t) = \langle \Psi(t) | x | \Psi(t) \rangle = \int d\vec{q} F(\vec{q}, t) \langle \vec{q} | x | \phi_i \rangle + \text{C.C} \quad (1.32)$$

We will consider only on-shell continuum-continuum scattering, which is relevant to HHG (off-shell scattering contributes to ATI), and we will write the the continuum components $F(\vec{q}, t)$ as a temporal integral over t' of function $G(\vec{q}, t')$. Since the harmonic strength X_{2K+1} is determined by

$$X_{2K+1} = \frac{w}{2\pi} \int_0^{2\pi/w} dt X(t) e^{iw(2K+1)t} \quad (1.33)$$

then from (1.32) we have

$$X_{2K+1} = \frac{w}{2\pi} \int_0^{2\pi/w} dt \int_0^t dt' \int d\vec{q} G(\vec{q}, t) \langle \vec{q} | x | \phi_i \rangle e^{iw(2K+1)t} + \text{C.C} \quad (1.34)$$

Equation (1.34) has the same structure and difficulty as (1.31). We will employ the same approach for the numerical evaluation of (1.34) and therefore will be in a position to determine accurately the HHG cutoff. *No such an accurate numerical attempt in the velocity gauge has been done before.* However, the computational work will be carried out in later work.

In Chapter (2) we will lay out the detailed theoretical background required for our formulation. In Chapter (3) we will present in detail our theoretical formulation. In Chapter (4) we will present the results of the numerical computations and finally Chapter (5) will contain discussions and conclusions.

Chapter 2

Theory I: Theoretical Background

We will look upon the problem of an atomic system interacting with strong laser fields within the framework of time dependent scattering theory. Throughout this chapter and the remainder of this work, the atomic system of units is used ($\hbar = m_e = |e| = 1$).

2.1 Basic Elements of Time Dependent Formal Scattering Theory

The state vector $\Psi(t)$ of a given physical system is assumed to satisfy the Schrödinger equation

$$i\frac{\partial}{\partial t}\Psi(t) = H\Psi(t) \quad (2.1)$$

H being the total hamiltonian operator. Furthermore, we assume that the Hamiltonian operator H can be split into two parts,

$$H = H_o + H_{\text{int}} \quad (2.2)$$

so that H_o represents the free hamiltonian of the system in the absence of interaction, and H_{int} represents the interaction hamiltonian between the system and the external field. It is

assumed that the Shrödinger equation for the free hamiltonian can be solved exactly and hence the state vector $\Psi_o(t)$ of the free hamiltonian is completely known. For the sake of simplicity, we assume that H is independent of time.

2.1.1 The Green Functions

In order to solve Eq. (2.1), we define four kinds of propagators, or Green's functions, by the equations

$$\left(i \frac{\partial}{\partial t} - H_o \right) G_o^\pm(t) = \mathbf{1} \delta(t) \tag{2.3}$$

$$\left(i \frac{\partial}{\partial t} - H \right) G^\pm(t) = \mathbf{1} \delta(t)$$

and the initial conditions

$$G_o^+(t) = G^+(t) = 0 \quad \text{for } t < 0 \tag{2.4}$$

$$G_o^-(t) = G^-(t) = 0 \quad \text{for } t > 0$$

Thus G_o^+ and G^+ are the *retarded* Green's functions and G_o^- and G^- *advanced* ones. In Eqs. (2.3), $\delta(t)$ stands for Dirac's delta function and $\mathbf{1}$ is the Identity operator. These equations are easily solved by writing the Fourier transforms of the Dirac delta function and the the Green's functions $G_o(t)$ and $G(t)$

$$\begin{aligned} \delta(t) &= \frac{1}{2\pi} \int_{-\infty}^{\infty} dw e^{iwt} \\ G_o(t) &= \frac{1}{2\pi} \int_{-\infty}^{\infty} dw \tilde{G}_o(w) e^{iwt} \\ G(t) &= \frac{1}{2\pi} \int_{-\infty}^{\infty} dw \tilde{G}(w) e^{iwt} \end{aligned}$$

Substituting in Eq. (2.3) gives

$$\begin{aligned} \tilde{G}_o(w) &= \frac{-1}{w + H_o} \\ \tilde{G}(w) &= \frac{-1}{w + H} \end{aligned}$$

and therefore we have the following integrals for $G_o(t)$ and $G(t)$

$$\begin{aligned} G_o(t) &= \frac{-1}{2\pi} \int_{-\infty}^{\infty} dw \frac{e^{iwt}}{w + H_o} \\ G(t) &= \frac{-1}{2\pi} \int_{-\infty}^{\infty} dw \frac{e^{iwt}}{w + H} \end{aligned}$$

Both integrals for G_o and G have simple poles at $w = -H_o$ and $w = -H$ respectively. To evaluate these integrals subject to the initial conditions given in Eq. (2.4), the poles can be displaced infinitesimally either into the upper half plane or the lower half plane. If the poles are displaced into the upper half plane then for $t < 0$, closing the contour into the lower half plane gives $G_o^{(+)}(t) = G^{(+)}(t) = 0$ and for $t > 0$ closing the contour into the upper half plane gives $G_o^{(+)} = -ie^{-iH_o t}$ and $G^{(+)} = -ie^{-iHt}$. Similarly, if the poles are displaced into the lower half plane, then for $t > 0$, closing the contours into the upper half plane gives $G_o^{(-)}(t) = G^{(-)}(t) = 0$ and for $t < 0$, closing the contour into the lower half plane gives $G_o^{(-)}(t) = ie^{-iH_o t}$ and $G^{(-)}(t) = ie^{-iHt}$. Thus, we can write

$$G_o^{(+)}(t) = -i\Theta(t) \exp(-iH_o t) \tag{2.5}$$

$$G_o^{(-)}(t) = i\Theta(-t) \exp(-iH_o t)$$

and

$$G^{(+)}(t) = -i\Theta(t) \exp(-iHt) \tag{2.6}$$

$$G^{(-)}(t) = i\Theta(-t) \exp(-iHt)$$

where $\Theta(t)$ is the Heviside step function.

From the defining equations (2.3), it is implied that $G_o^{(\pm)}$ commutes with H_o and similarly $G^{(\pm)}$ with H . Since the operators H_o and H are Hermitian, it follows that

$$G_o^{(+)}(t)^\dagger = G_o^{(-)}(-t) \tag{2.7}$$

$$G^{(+)}(t)^\dagger = G^{(-)}(-t)$$

which are obvious in Eqs. (2.5) and (2.6).

Since $\Psi_o(t)$ is explicitly known and hence $G_o^{(\pm)}$, then we may write $G^{(\pm)}$ in terms of $G_o^{(\pm)}$:

$$G^{(\pm)}(t-t') = G_o^{(\pm)}(t-t') + \int dt'' G_o^{(\pm)}(t-t'') H_{\text{int}} G^{(\pm)}(t''-t') \quad (2.8)$$

or

$$G^{(\pm)}(t-t') = G_o^{(\pm)}(t-t') + \int dt'' G^{(\pm)}(t-t'') H_{\text{int}} G_o^{(\pm)}(t''-t') \quad (2.9)$$

The limits of the integrals in eqs. (2.8) and (2.9) depend upon their use for $G_o^{(+)}$ or $G_o^{(-)}$, so that convergence questions in them do not arise.

The state vector $\Psi_o(t)$ satisfies the free Schrödinger equation

$$i \frac{\partial}{\partial t} \Psi_o = H_o(t) \Psi_o(t) \quad (2.10)$$

Then the operator $G_o^{(+)}$ allows us to express the state vector $\Psi_o(t')$ for any time $t' > t$, in terms of its value at $t' = t$,

$$\Psi_o(t') = i G_o^{(+)}(t' - t) \Psi_o(t) \quad (2.11)$$

It is easy to verify explicitly that Ψ_o satisfies Eq. (2.10) for $t' > t$ and the vector $\Psi_o(t')$ on the left approaches the vector $\Psi_o(t)$ on the right when $t' \rightarrow t^+$. This is because

$$\lim_{t \rightarrow 0^+} G_o^{(+)}(t) = -i \mathbf{1} \quad (2.12)$$

as well as

$$\lim_{t \rightarrow 0^+} G^{(+)}(t) = -i \mathbf{1} \quad (2.13)$$

and

$$\lim_{t \rightarrow 0^-} G_o^{(-)}(t) = \lim_{t \rightarrow 0^-} G^{(-)}(t) = i \mathbf{1} \quad (2.14)$$

Similarly we have for $t' > t$

$$\Psi(t') = i G^{(+)}(t' - t) \Psi(t) \quad (2.15)$$

and for $t' < t$

$$\Psi_o(t') = -i G_o^{(-)}(t' - t) \Psi_o(t) \quad (2.16)$$

$$\Psi(t') = -i G^{(-)}(t' - t) \Psi(t)$$

The operators $G_o^{(+)}$ and $G^{(+)}$ thus describe the propagation of waves subject to the Hamiltonians H_o and H respectively in the future, and $G_o^{(-)}$ and $G^{(-)}$ in the past.

2.1.2 In and Out States

Now we are in a position to introduce the *in* state Ψ_{in} and the *out* state Ψ_{out} . First let us define

$$\Psi_o \equiv iG_o^{(+)}(t-t')\Psi(t') \quad (2.17)$$

This is a state vector whose time development for $t > t'$ is governed by the free Hamiltonian H_o but which at time t_o was equal to the to $\Psi(t_o)$. Let us now allow $t' \rightarrow -\infty$. This defines the state

$$\Psi_{\text{in}} \equiv \lim_{t' \rightarrow -\infty} iG_o^{(+)}(t-t')\Psi(t') \quad (2.18)$$

Then Ψ_{in} is a free state vector. It is a state which at all times develops according H_o , in which the system does not interact with the external field, but which in the remote past was equal to the exact state vector of the complete interacting system with the external field. In the remote past the system was prepared in the state Ψ_{in} , since then it is assumed that the interaction between the system and the external field can be neglected.

Now because of the defining Eq. (2.3) and since $G_o^{(+)}$ and H_o commute we get

$$\begin{aligned} i\frac{\partial}{\partial t'} \left[G_o^{(+)}(t-t')\Psi(t') \right] &= -i\frac{\partial}{\partial t} G_o^{(+)}(t-t')\Psi(t') + G_o^{(+)}(t-t')i\frac{\partial}{\partial t'} \Psi(t') \\ &= -\delta(t-t')\Psi(t') + G_o^{(+)}(t-t')H_{\text{int}}\Psi(t') \end{aligned}$$

integrating from $t' = -\infty$ to $+\infty$ and using Eq. (2.18) we get

$$\Psi(t) = \Psi_{\text{in}}(t) + \int_{-\infty}^t dt' G_o^{(+)}(t-t')H_{\text{int}}\Psi(t') \quad (2.19)$$

as an integral equation satisfied by $\Psi(t)$. Of course since $G_o^{(+)}(t-t')$ is nonzero only when $t > t'$ then the upper limit of integration is set equal to t . It is clear from Eq. (2.19) that in the limit $t \rightarrow -\infty$, $\Psi = \Psi_{\text{in}}$, that it is to say, in the remote past the system was noninteracting with the external field and was prepared to be in the state Ψ_{in} .

In a similar fashion we can define

$$\Psi_{\text{out}}(t) = - \lim_{t' \rightarrow -\infty} iG_o^{(-)}(t-t')\Psi(t') \quad (2.20)$$

which is a free state vector whose time development is governed by H_o , equal to the complete state Ψ in the remote future. Similar to Eq. (2.19) we then get

$$\Psi(t) = \Psi_{\text{out}}(t) + \int_t^\infty dt' G^{(-)}(t-t') H_{\text{int}} \Psi(t') \quad (2.21)$$

where the lower limit of integration is set equal to t because the advanced Green's function $G^{(-)}$ is non zero only when $t' > t$. Again in the limit $t \rightarrow \infty$, $\Psi = \Psi_{\text{out}}$, that is to say, in the remote future the system is no longer interacting with the external field, and therefore would be in the free state Ψ_{out} .

In a reversed manner, one can define

$$\Psi(t) = \imath G^{(+)}(t-t') \Psi_o(t') \quad (2.22)$$

The state vector $\Psi(t)$ develops in time according to the full hamiltonian, for all times $t > t'$, and at $t = t'$ it was equal to $\Psi(t_o)$. Hence, if we let $t' \rightarrow \pm\infty$, we must obtain

$$\Psi(t) = \lim_{t' \rightarrow -\infty} \imath G^{(+)}(t-t') \Psi_{\text{in}}(t') \quad (2.23)$$

$$\Psi(t) = \lim_{t' \rightarrow \infty} \imath G^{(-)}(t-t') \Psi_{\text{out}}(t')$$

and as we did in the derivation of Eqs. (2.19) and (2.21)

$$\Psi(t) = \Psi_{\text{in}} + \int_{-\infty}^t dt' G^{(+)}(t-t') H_{\text{int}} \Psi_{\text{in}}(t') \quad (2.24)$$

$$\Psi(t) = \Psi_{\text{out}} + \int_t^\infty dt' G^{(-)}(t-t') H_{\text{int}} \Psi_{\text{out}}(t') \quad (2.25)$$

Let us re-examine Eqs. (2.19) and (2.21). In an actual experimental situation Ψ_{in} contains all the information on how the the system was prepared in the remote past. This information refers to set of quantum numbers $\{\alpha\}$, or eigenvalues of dynamical variables, which commute with H_o and can thus be specified in a free state Ψ_o . Therefore, a complete state thus determined is labeled by the same quantum numbers $\{\alpha\}$ of Ψ_{in} and is denoted by $\Psi^{(+)}(\alpha, t)$. Therefore, the state $\Psi^{(+)}(\alpha, t)$ satisfies

$$\Psi^{(+)}(\alpha, t) = \Psi_{\text{in}}(\alpha, t) + \int_{-\infty}^t dt' G_o^{(+)}(t-t') H_{\text{int}} \Psi^{(+)}(\alpha, t') \quad (2.26)$$

It was *controlled*, so to speak, in the remote past as indicated by the label $\{\alpha\}$.

In the distant future $\Psi^{(+)}(\alpha, t)$ will be essentially a free state. It contains in addition to the controlled part Ψ_{in} , an unknown part of outgoing scattered waves.

In a similar fashion, we can define a complete state by its controlled behavior in the remote future. Such a state is denoted $\Psi^{(-)}(\beta, t)$. Its label $\{\beta\}$ refers to the quantum numbers of $\Psi_{\text{out}}(\beta, t)$. They must be of the same kind as before, i.e, must commute with H_0 . The state $\Psi^{(-)}(\beta, t)$ satisfies

$$\Psi^{(-)}(\beta, t) = \Psi_{\text{out}}(\beta, t) + \int_t^\infty dt' G_0^{(-)}(t - t') H_{\text{int}} \Psi^{(-)}(\beta, t') \quad (2.27)$$

In the remote past $\Psi^{(-)}(\beta, t)$ must have been a free state where it differs from Ψ_{out} by an unknown amount of incoming waves.

2.1.3 The S Matrix

In a scattering experiment the system first is prepared into the free state Ψ_{in} . Then the interaction is slowly turned on where now the system will evolve into the complete state Ψ . Finally, the interaction will be turned off asymptotically and the system will go over into the free state Ψ_{out} . Therefore, it is of interest to express the *out* state of a state vector in terms of its *in* state.

The free state vectors Ψ_{in} and Ψ_{out} evolve according to

$$\Psi_{\text{in}}(t') = -i G_0^{(-)}(t' - t) \Psi_{\text{in}}(t) \quad \text{for } t > t' \quad (2.28)$$

$$\Psi_{\text{out}}(t') = i G_0^{(+)}(t' - t) \Psi_{\text{out}}(t) \quad \text{for } t < t' \quad (2.29)$$

substituting Eq. (2.28) into Eq. (2.24) we obtain

$$\Psi(t) = \Omega^{(+)} \Psi_{\text{in}}(t) \quad (2.30)$$

where, $\Omega^{(+)}$ is called the Møller wave operator and is given by

$$\begin{aligned} \Omega^{(+)} &= 1 - i \int_{-\infty}^t dt' G^{(+)}(t - t') H_{\text{int}} G_0^{(-)}(t' - t) \\ &= 1 - i \int_{-\infty}^0 d\tau G^{(+)}(-\tau) H_{\text{int}} G_0^{(-)}(\tau) \\ &= 1 - i \int_{-\infty}^{\infty} d\tau G^{(+)}(-\tau) H_{\text{int}} G_0^{(-)}(\tau) \end{aligned} \quad (2.31)$$

where we set $\tau = t' - t$ and it is immaterial to extend the upper limit of integration to $+\infty$. Thus the Møller wave operator is a time-independent operator which converts the free state $\Psi_{\text{in}}(t)$ directly into that complete state $\Psi(t)$ which corresponds to it in the sense that it was essentially equal to it in the remote past.

Similarly, inserting Eq. (2.29) into Eq. (2.25) we obtain

$$\Psi(t) = \Omega^{(-)}\Psi_{\text{out}}(t) \quad (2.32)$$

where, $\Omega^{(-)}$ is given by

$$\Omega^{(-)} = 1 + i \int_{-\infty}^{\infty} d\tau G^{(-)}(-\tau) H_{\text{int}} G_0^{(+)}(\tau) \quad (2.33)$$

Applying the same procedure to Eqs. (2.19) and (2.21) by inserting into them Eqs. (2.16) and (2.15) respectively, using Eq. (2.7) and the hermiticity of H_{int} , we obtain

$$\Psi_{\text{in}}(t) = \Omega^{(+)\dagger}\Psi(t) \quad (2.34)$$

$$\Psi_{\text{out}}(t) = \Omega^{(-)\dagger}\Psi(t) \quad (2.35)$$

multiplying Eq. (2.30) by $\Omega^{(-)\dagger}$ and using Eq. (2.35) we finally arrive at the sought after relationship

$$\Psi_{\text{out}}(t) = \Omega^{(-)\dagger}\Omega^{(+)}\Psi_{\text{in}}(t) \quad (2.36)$$

In a likewise fashion, multiplying Eq. (2.32) by $\Omega^{(+)\dagger}$ and using Eq. (2.34) we obtain

$$\begin{aligned} \Psi_{\text{in}}(t) &= \Omega^{(+)\dagger}\Omega^{(-)}\Psi_{\text{out}}(t) \\ &= S^\dagger\Psi_{\text{out}}(t) \end{aligned} \quad (2.37)$$

According to Eq. (2.36), we can define the scattering operator

$$S = \Omega^{(-)\dagger}\Omega^{(+)} \quad (2.38)$$

The matrix of S on the basis of the free states of the Hamiltonian H_0 is called the S matrix. Since the sets $\{\Psi_{\text{in}}\}$ and $\{\Psi_{\text{out}}\}$ are assumed to be complete, we deduce from Eq. (2.36) and (2.37) that S is unitary,

$$S^\dagger S = S S^\dagger = 1 \quad (2.39)$$

The Fundamental Question of Scattering Theory

Now we are in a position to answer the Fundamental question of scattering: If the system is described by the state vector $\Psi^{(+)}(\alpha, t)$, which is known to have been in the controlled state $\Psi_{\text{in}}(\alpha, t) = \Psi_{\text{o}}(\alpha, t)$ in the remote past, what is the probability of finding it in the state $\Psi^{(-)}(\beta, t)$, which is known to go over into the controlled state $\Psi_{\text{out}}(\beta, t) = \Psi_{\text{o}}(\beta, t)$ in the remote future? Its probability amplitude is given by the S matrix element

$$\begin{aligned}
 S_{\beta\alpha} &= \langle \Psi^{(-)}(\beta, t) | \Psi^{(+)}(\alpha, t) \rangle & (2.40) \\
 &= \langle \Omega^{(-)}\Psi_{\text{out}}(\beta, t) | \Omega^{(+)}\Psi_{\text{in}}(\alpha, t) \rangle \\
 &= \langle \Psi_{\text{out}}(\beta, t) | \Omega^{(-)\dagger}\Omega^{(+)}\Psi_{\text{in}}(\alpha, t) \rangle \\
 &= \langle \Psi_{\text{out}}(\beta, t) | S\Psi_{\text{in}}(\alpha, t) \rangle \\
 &= \langle \Psi_{\text{o}}(\beta, t) | S\Psi_{\text{o}}(\alpha, t) \rangle & (2.41)
 \end{aligned}$$

The above question can be asked in slightly different way: If in the remote past the system was in the controlled state $\Psi_{\text{in}}(\alpha, t) = \Psi_{\text{o}}(\alpha, t)$, so now it is in the state $\Psi^{(+)}(\alpha, t)$, then, what is the probability for finding it in the state $\Psi_{\text{o}}(\beta, t)$ in the distant future. The probability amplitude is given by letting $t \rightarrow \infty$ in Eq. (2.40)

$$\begin{aligned}
 S_{\beta\alpha} &= \lim_{t \rightarrow \infty} \langle \Psi^{(-)}(\beta, t) | \Psi^{(+)}(\alpha, t) \rangle \\
 &= \langle \Psi_{\text{o}}(\beta, t) | \Psi_{\text{out}}(\alpha, t) \rangle \\
 &= \langle \Psi_{\text{o}}(\beta, t) | \Omega^{(-)\dagger}\Omega^{(+)}\Psi_{\text{in}}(\alpha, t) \rangle \\
 &= \langle \Psi_{\text{o}}(\beta, t) | S\Psi_{\text{o}}(\alpha, t) \rangle & (2.42)
 \end{aligned}$$

where according to Eq. (2.27) $\lim_{t \rightarrow \infty} \Psi^{(-)}(\beta, t) = \Psi_{\text{out}}(\beta, t) = \Psi_{\text{o}}(\beta, t)$ and since for asymptotic times $G^{(+)} \rightarrow G_{\text{o}}^{(+)}$ and therefore $\Psi^{(+)} = \Psi_{\text{out}}$. The answer, of course, is the same. This is what is called the *time direct* Scattering matrix.

The same question can be asked yet in another manner: If in the distant future the system is in the controlled state $\Psi_{\text{out}}(\beta, t) = \Psi_{\text{o}}(\beta, t)$, which is evolved from the state $\Psi^{(-)}(\beta, t)$, then what is the probability that the system would have been in the state $\Psi_{\text{in}}(\alpha, t) = \Psi_{\text{o}}(\alpha, t)$ in the remote past. The probability amplitude is given by letting

$t \rightarrow -\infty$ in Eq. (2.40)

$$\begin{aligned}
 S_{\beta\alpha} &= \lim_{t \rightarrow -\infty} \langle \Psi^{(-)}(\beta, t) | \Psi^{(+)}(\alpha, t) \rangle \\
 &= \langle \Psi_{\text{in}}(\beta, t) | \Psi_{\text{o}}(\alpha, t) \rangle \\
 &= \langle S^\dagger \Psi_{\text{out}}(\beta, t) | \Psi_{\text{o}}(\alpha, t) \rangle \\
 &= \langle \Psi_{\text{o}}(\beta, t) | S \Psi_{\text{o}}(\alpha, t) \rangle
 \end{aligned} \tag{2.43}$$

where according to Eq. (2.26) $\lim_{t \rightarrow -\infty} \Psi^{(+)}(\alpha, t) = \Psi_{\text{in}}(\alpha, t) = \Psi_{\text{o}}(\alpha, t)$ and since for negative asymptotic times $G^{(-)} \rightarrow G_{\text{o}}^{(-)}$ and therefore $\Psi^{(-)} = \Psi_{\text{in}}$. The answer is again the same. This is what is called the *time reverse* Scattering matrix.

2.2 S-Matrix Formalism with Two Potentials

The usual S-matrix formalism, introduced above, for transitions induced in a system will be extended here to the case where there are two distinct independent interaction terms. Initially, both interactions will be considered to be of equivalent importance, and both can be time dependent. This is the case of an atomic system in strong light field. Within the single active electron model, the atomic electron is under the influence of both the atomic potential and the strong light field, where both of the interactions are of equivalent importance (it is not the case for weak light fields). Distinctions between the interaction terms will be introduced as the formalism is developed.

The system under consideration is described in full by the the Schrödinger equation

$$\left(i \frac{\partial}{\partial t} - H_{\text{o}} - V_{\text{L}} - V_{\text{A}} \right) \Psi = 0 \tag{2.44}$$

where H_{o} now is the kinetic energy operator, and V_{L} and V_{A} can both be time dependent. $H_{\text{o}}, V_{\text{L}}, V_{\text{A}}$ are of course Hilbert space operators, Ψ is a state vector in Hilbert space. It is presumed that the solution vectors Ψ_{L} and Ψ_{A} to the equations

$$\left(i \frac{\partial}{\partial t} - H_{\text{o}} - V_{\text{L}} \right) \Psi_{\text{L}} = 0 \tag{2.45}$$

$$\left(i \frac{\partial}{\partial t} - H_{\text{o}} - V_{\text{A}} \right) \Psi_{\text{A}} = 0 \tag{2.46}$$

are known. The corresponding Green's operators satisfy the equations

$$\left(\imath \frac{\partial}{\partial t} - H_o - V_L \right) G_L(t, t') = 1\delta(t - t') \quad (2.47)$$

$$\left(\imath \frac{\partial}{\partial t} - H_o - V_A \right) G_A(t, t') = 1\delta(t - t') \quad (2.48)$$

where 1 is the unit operator of the Hilbert space. Rather than writing the solutions $G_L^{(\pm)}$ and G_A^{\pm} in a symbolic form, as we did in Eqs. (2.5) and (2.6), we write for example $G_L^{(\pm)}$ as

$$G_L^{(+)}(t, t') = -\imath\Theta(t - t') \sum_j |L, j, t\rangle \langle L, j, t'| \quad (2.49)$$

for the retarded Green's function and

$$\begin{aligned} G_L^{(-)}(t, t') &= G^{(+)\dagger}(t', t) \\ &= \imath\Theta(t' - t) \sum_j |L, j, t\rangle \langle L, j, t'| \end{aligned} \quad (2.50)$$

for the advanced Green's function and where, for convenience, Dirac bra-ket notation is used for the state vectors with the correspondence

$$\Psi_{Lj}(t) \longleftrightarrow |L, j, t\rangle \quad (2.51)$$

and the index j represents all the quantum numbers which define the state. It is easy to verify that $G_L^{(\pm)}$ given by Eqs. (2.49) and (2.50) do indeed satisfy Eq. (2.47). The retarded and advanced Green's operator $G_A^{(\pm)}$ are, of course, of the same form as Eqs. (2.49) and (2.50). The action of the Green's operator on a state vector is seen to be

$$G^{(+)}(t, t')\Psi_L(t') = -\imath\Theta(t - t')\Psi_L(t) \quad (2.52)$$

$$G^{(-)}(t, t')\Psi_L(t') = \imath\Theta(t' - t)\Psi_L(t) \quad (2.53)$$

The solution of Eq. (2.44) is given either as

$$\Psi^{(\pm)}(t) = \Psi_L(t) + \int dt' G_L^{(\pm)} V_A(t') \Psi^{(\pm)}(t') \quad (2.54)$$

or as

$$\Psi^{(\pm)}(t) = \Psi_A(t) + \int dt' G_A^{(\pm)} V_L(t') \Psi^{(\pm)}(t') \quad (2.55)$$

where it is understood that $\Psi_L(t)$ in Eq. (2.54) and $\Psi_A(t)$ in Eq. (2.55) are either *in* state or *out* state.

Up to now, the interactions V_L and V_A have been treated entirely on equal footing. Now it will be supposed that V_L is turned off at asymptotic times, but V_A is not; and it is the transitions caused by V_L which are to be calculated.

As we outlined in section 2.1.3, the transition S matrix may be then expressed either in terms of the $\Psi^{(+)}$ (time direct S matrix) as

$$S_{fi} = \lim_{t \rightarrow \infty} \langle \Psi_{A_f} | \Psi_i^{(+)} \rangle \quad (2.56)$$

or in terms of $\Psi^{(-)}$ (time reverse S matrix) as

$$S_{fi} = \lim_{t \rightarrow -\infty} \langle \Psi_f^{(-)} | \Psi_{A_i} \rangle \quad (2.57)$$

where the subscripts i and f represent initial and final conditions, respectively. Again, the physical meaning of Eq. (2.56) is that the S matrix is the probability amplitude that the complete state of the system $\Psi^{(+)}$ (including both V_L and V_A) will, at infinite time, be in some particular state of the system in which only V_A is present.

The time direct S matrix will be examined first. Direct substitution for $\Psi_i^{(+)}$ by the expression given by Eq. (2.55) gives

$$\begin{aligned} S_{fi} &= \lim_{t \rightarrow \infty} \langle \Psi_{A_f} | \Psi_{A_i} \rangle + \lim_{t \rightarrow \infty} \int_{-\infty}^t dt' \langle \Psi_{A_f}(t) | G_A^{(+)}(t, t') V_L(t') \Psi_i^{(+)}(t') \rangle \\ &= \delta_{fi} + \lim_{t \rightarrow \infty} \int_{-\infty}^t dt' \langle G_A^{(-)}(t', t) \Psi_{A_f}(t) | V_L(t') \Psi_i^{(+)}(t') \rangle \end{aligned}$$

Using Eq. (2.53) and $\lim_{t \rightarrow \infty} \Theta(t - t') = 1$, we obtain

$$(S - 1)_{fi} = -i \int_{-\infty}^{\infty} dt' \langle \Psi_{A_f} | V_L \Psi_i^{(+)} \rangle_{t'} \quad (2.58)$$

where the subscript t' on the the inner product in the integrand means that all components of that product have the argument t' .

Now the time reverse S matrix will be examined. Direct substitution for $\Psi_f^{(-)}$ by the expression given by Eq. (2.55) gives

$$\begin{aligned} S_{fi} &= \lim_{t \rightarrow -\infty} \langle \Psi_{A_f} | \Psi_{A_i} \rangle + \lim_{t \rightarrow -\infty} \int_t^{\infty} dt' \langle G_A^{(-)}(t, t') V_L(t') \Psi_f^{(-)}(t') | \Psi_{A_i}(t) \rangle \\ &= \delta_{fi} + \lim_{t \rightarrow -\infty} \int_t^{\infty} dt' \langle \Psi_f^{(-)}(t') | V_L(t') G_A^{(+)}(t' - t) \Psi_{A_i}(t) \rangle \end{aligned}$$

Using Eq. (2.52) and $\lim_{t \rightarrow -\infty} \Theta(t' - t) = 1$, we obtain

$$(S - 1)_{\text{fi}} = -i \int_{-\infty}^{\infty} dt' \langle \Psi_{\text{f}}^{(-)} | V_{\text{L}} \Psi_{\text{A}_i} \rangle_{t'} \quad (2.59)$$

2.3 The Volkov Wave Function

The Volkov wave function is the solution of the Schrödinger equation for a free electron in an electromagnetic field. Depending on the choice of gauge, and within the dipole approximation, the Schrödinger equation can be written either in the *length gauge* as

$$\left(i \frac{\partial}{\partial t} - \frac{1}{2} P^2 - \vec{E} \cdot \vec{r} \right) \Psi_{\text{L}} = 0 \quad (2.60)$$

or in the *velocity gauge* as

$$\left(i \frac{\partial}{\partial t} - \frac{1}{2} P^2 - \frac{1}{c} \vec{A} \cdot \vec{P} - \frac{A^2}{2c^2} \right) \Psi_{\text{V}} = 0 \quad (2.61)$$

where the electric field $\vec{E} = -\frac{1}{c} \frac{\partial \vec{A}}{\partial t}$, \vec{A} is the vector potential of the electromagnetic field, c is the speed of light and $\vec{P} = -i \vec{\nabla}$ is the canonical momentum operator.

To find these solutions, the Schrödinger equation in the *length gauge* will be examined first. Let us carry out a unitary transformation and write

$$\Psi_{\text{L}} = e^{\frac{i}{c} \vec{A} \cdot \vec{r}} \Phi \quad (2.62)$$

Substituting in Eq. (2.60) and using $\vec{E} = -\frac{1}{c} \frac{\partial \vec{A}}{\partial t}$, we obtain

$$\left(i \frac{\partial}{\partial t} - e^{\frac{-i}{c} \vec{A} \cdot \vec{r}} \frac{1}{2} P^2 e^{\frac{i}{c} \vec{A} \cdot \vec{r}} \right) \Phi = 0 \quad (2.63)$$

Within the dipole approximation, it is assumed that the vector potential \vec{A} has no spatial dependence and therefore using the quantum mechanical rule for the transformation of operators [69]

$$e^{\frac{-i}{c} \vec{A} \cdot \vec{r}} \frac{1}{2} P^2 e^{\frac{i}{c} \vec{A} \cdot \vec{r}} \equiv \frac{1}{2} \left(\vec{P} + \frac{1}{c} \vec{A} \right)^2 \quad (2.64)$$

we finally get

$$\left(i \frac{\partial}{\partial t} - \frac{1}{2} P^2 - \frac{1}{c} \vec{A} \cdot \vec{P} - \frac{A^2}{2c^2} \right) \Phi = 0 \quad (2.65)$$

comparing Eqs. (2.65) and (2.61) and from Eq. (2.62) we deduce immediately that

$$\Psi_{\text{L}} = e^{\frac{i}{c}\vec{A}\cdot\vec{r}} \Psi_{\text{V}} \quad (2.66)$$

Therefore once we obtain the solution Ψ_{V} then Ψ_{L} is obtained through a unitary transformation as given by Eq.(2.66).

Next we examine the Schrödinger equation in the *velocity gauge*. In the laboratory frame the free electron is sitting in the oscillating electromagnetic field. However if we carry a transformation to a frame that oscillates in phase with the electromagnetic field, then the electron in that frame is a plane wave. This is the essence of the Henneberger transformation [70]. Thus we write

$$\Psi_{\text{V}} = e^{-i \int_{-\infty}^t dt' \left(\frac{1}{c}\vec{A}(t')\cdot\vec{P} + \frac{A^2(t')}{2c^2} \right)} \tilde{\Phi} \quad (2.67)$$

substituting in Eq. (2.61) we get

$$\left(i \frac{\partial}{\partial t} - \frac{1}{2} P^2 \right) \tilde{\Phi} = 0 \quad (2.68)$$

Thus using the Dirac bra-ket notation we write

$$| \Psi_{\text{V}} \rangle = e^{-iS(\vec{k},t)} | \vec{k} \rangle \quad (2.69)$$

and therefore from Eq. (2.66) we write

$$| \Psi_{\text{L}} \rangle = e^{-iS(\vec{k},t)} | \vec{k} + \frac{1}{c}\vec{A} \rangle \quad (2.70)$$

where $S(\vec{k}, t)$ is the semiclassical action for a free electron in an electromagnetic field

$$S(\vec{k}, t) = \int_{-\infty}^t dt' \left[\vec{k} + \frac{1}{c}\vec{A}(t') \right]^2 \quad (2.71)$$

with the plane waves $| \vec{k} \rangle$ and $| \vec{k} + \frac{1}{c}\vec{A} \rangle$

$$\begin{aligned} \langle \vec{r} | \vec{k} \rangle &= \frac{1}{(2\pi)^{\frac{3}{2}}} e^{i\vec{k}\cdot\vec{r}} \\ \langle \vec{r} | \vec{k} + \frac{1}{c}\vec{A} \rangle &= \frac{1}{(2\pi)^{\frac{3}{2}}} e^{i(\vec{k} + \frac{1}{c}\vec{A})\cdot\vec{r}} \end{aligned}$$

2.4 The Keldysh -Faisal- Reiss (KFR) Theory for Laser Induced Ionization: The Direct Electrons

The goal is to find a suitable approximation to the probability amplitude for detecting an above threshold ionization (ATI) electron with drift momentum \vec{K} that originates from the laser irradiation of an atom that was in its ground state $|\phi_i\rangle$ before the laser pulse arrived. As outlined in section (2.2), the S matrix to describe the ionization process can be written in general in terms of the *time reverse* S matrix as

$$S_{fi} = \lim_{t \rightarrow -\infty} \langle \Psi_f^{(-)} | \phi_i \rangle \quad (2.72)$$

where $\Psi_f^{(-)}$ is the final out-state of the system containing the complete effects of the electromagnetic field as well as the binding potential, while ϕ_i is the initial state of the unperturbed atomic system with no field present. Alternatively, one can use the *time direct* S matrix

$$S_{fi} = \lim_{t \rightarrow \infty} \langle \phi_f | \Psi_i^{(+)} \rangle \quad (2.73)$$

The form given in terms of the *time reverse* S matrix is more convenient than the alternative *time direct* form. This is because ϕ_i in Eq. (2.72) is the initial, unperturbed, bound state, which is unique and well-known; whereas ϕ_f would be one of a set of continuum states. Furthermore, $\Psi_f^{(-)}$ in Eq. (2.72) can reasonably be assumed to be dominated by the applied field, whereas no such assumption can be made for $\Psi_i^{(+)}$. As shown in the previous section, Eq. (2.72) can be written as

$$(S - 1)_{fi} = -i \int_{-\infty}^{\infty} dt' \langle \Psi_f^{(-)} | V_L \phi_i \rangle_{t'} \quad (2.74)$$

where V_L represents the interaction potential due to the applied laser field, and as stated earlier, the subscript t' on the scalar product means that all factors in the product depend on t' . Eq. (2.74) is an exact equation. No exact analytic expression for $\Psi_f^{(-)}$ is known. After ionization the electron is still under the combined effect of both the intense laser field and the long-range atomic Coulomb potential. However, for intense laser fields, if the residual effects of the atomic Coulomb potential are ignored, then the ionized free electron will be dominated by the intense laser field. Therefore $\Psi_f^{(-)}$ will be adequately replaced by the

state vector of a free electron in the presence of the electromagnetic field; i.e., the Volkov state vector $\Psi_{\vec{k}}^{(v)}$. This is exactly the Keldysh approximation [3]. With this approximation in mind, Eq. (2.74) for the scattering matrix takes the approximate form

$$(S - 1)_{\text{fi}} \approx -i \int_{-\infty}^{\infty} dt' \langle \Psi_{\vec{k}}^{(v)} | V_{\text{L}} \phi_i \rangle_{t'} \quad (2.75)$$

This approximate expression for the S matrix is what is called the Keldysh-Faisal-Reiss (KFR) theory and also coined the strong field approximation (SFA).

To evaluate the approximate expression for the S matrix given in Eq. (2.75), the applied electromagnetic field will be treated in the *velocity gauge*

$$V_{\text{L}}(t) = \frac{1}{c} \vec{A} \cdot (-i\vec{\nabla}) + \frac{A^2}{2c^2} \quad (2.76)$$

and therefore as given by Eq. (2.69), the Volkov state, using Dirac bra-ket notation

$$| \Psi_{\vec{k}}^{(v)} \rangle = e^{-iS(\vec{k}, t)} | \vec{k} \rangle \quad (2.77)$$

where $S(\vec{k}, t)$ is the semiclassical action for a free electron in the presence of the radiation field

$$S(\vec{k}, t) = \frac{1}{2} \int_{-\infty}^t dt' [\vec{k} + \frac{1}{c} A(t')]^2 \quad (2.78)$$

Notice that the Volkov state is an eigenfunction of the $V_{\text{L}}(t)$ operator,

$$V_{\text{L}}(t) | \Psi_{\vec{k}}^{(v)} \rangle = V_{\text{L}}(\vec{k}, t) | \Psi_{\vec{k}}^{(v)} \rangle \quad (2.79)$$

The initial-state wave function ϕ_i is a stationary bound state,

$$| \phi_i(t) \rangle = | \phi_i \rangle e^{-iE_i t} \quad (2.80)$$

Since V_{L} is a Hermitian operator, and using Eq. (2.79) the S matrix expression in Eq. (2.75) can be written as

$$\begin{aligned} (S - 1)_{\text{fi}} &= -i \int_{-\infty}^{\infty} dt \langle V_{\text{L}} \Psi_{\vec{k}}^{(v)} | \phi_i \rangle_t \\ &= -i \int_{-\infty}^{\infty} dt V_{\text{L}}(\vec{k}, t) \langle \Psi_{\vec{k}}^{(v)} | \phi_i \rangle_t \\ &= -i \int_{-\infty}^{\infty} dt \left(\dot{S}(\vec{k}, t) - \frac{k^2}{2} \right) \langle \Psi_{\vec{k}}^{(v)} | \phi_i \rangle_t \end{aligned} \quad (2.81)$$

where, $\dot{S} = \frac{\partial S}{\partial t}$. using Eqs. (2.77) and (2.80) we get

$$\begin{aligned} (S - 1)_{\text{fi}} &= -i \langle \vec{k} | \phi_i(\vec{r}) \rangle \int_{-\infty}^{\infty} dt e^{i(\frac{k^2}{2} - E_i)t} V_L(\vec{k}, t) e^{i \int_{-\infty}^t dt' V_L(\vec{k}, t')} \\ &= -i \langle \vec{k} | \phi_i(\vec{r}) \rangle \int_{-\infty}^{\infty} dt e^{iS(\vec{k}, t)} (\dot{S}(\vec{k}, t) - \frac{k^2}{2}) e^{-iE_i t} \end{aligned} \quad (2.82)$$

The integral over t can be done by carrying out integration by parts. This leads to an integrated part to be evaluated at $t = \pm\infty$.

$$\lim_{t \rightarrow \infty} \left[e^{i(\frac{k^2}{2} - E_i)t} e^{i \int_{-\infty}^t dt' V_L(\vec{k}, t')} \right]_{-t}^t$$

For a periodic \vec{A} , V_L is the sum of two terms; one is periodic and thus has a Fourier series and the other is a constant $= U_p = \frac{A_0^2}{4c^2}$, where U_p is the ponderomotive energy and A_0 is the amplitude of the $\vec{A}(t)$. This leads to

$$\lim_{t \rightarrow \infty} \left[e^{i(\frac{k^2}{2} - E_i)t} e^{i \int_{-\infty}^t dt' V_L(\vec{k}, t')} \right]_{-t}^t = \sum_{n=-\infty}^{\infty} f_n \lim_{t \rightarrow \infty} \left[e^{i(\frac{k^2}{2} - E_i - nw + U_p)t} \right]_{-t}^t$$

where f_n are Fourier components of the periodic function, and w is the frequency of the field. Since

$$\begin{aligned} \lim_{t \rightarrow \infty} \left(e^{i(\frac{k^2}{2} - E_i - nw + U_p)t} \right)_{-t}^t &= i \left(\frac{k^2}{2} - E_i - nw + U_p \right) \int_{-\infty}^{\infty} dt e^{i(\frac{k^2}{2} - E_i - nw + U_p)t} \\ &= 2\pi i \left(\frac{k^2}{2} - E_i - nw + U_p \right) \delta \left(\frac{k^2}{2} - E_i - nw + U_p \right) \\ &= 0 \end{aligned}$$

thus Eq. (2.82) now reads

$$(S - 1)_{\text{fi}} = i \langle \vec{k} | \phi_i \rangle \int_{-\infty}^{\infty} dt (E_k - E_i) e^{i(E_k - E_i + U_p)t} e^{i(S(\vec{k}, t) - E_k t - U_p t)} \quad (2.83)$$

where $E_k = \frac{k^2}{2}$. Now, as we explained above, $S(\vec{k}, t) - E_k t - U_p t$ is a periodic function of t with period $\frac{2\pi}{w}$. Therefore we can write

$$e^{i(S(\vec{k}, t) - E_k t - U_p t)} = \sum_{n=-\infty}^{\infty} f_n e^{-inwt} \quad (2.84)$$

and so Eq. (2.82) for the S matrix becomes

$$\begin{aligned}
 (S - 1)_{\text{fi}} &= \iota \langle \vec{k} | \phi_i \rangle (E_k + E_B) \sum_{n=n_o}^{\infty} \int_{-\infty}^{\infty} dt f_n e^{\iota(E_k + E_B + U_p - nw)t} \\
 &= 2\pi\iota \langle \vec{k} | \phi_i \rangle \sum_{n=n_o}^{\infty} (E_k + E_B) \delta(E_k + E_B + U_p - nw) f_n
 \end{aligned} \tag{2.85}$$

where $E_B = -E_i$ is the positive binding of the initial state and n_o is the minimum number of photons required for threshold ionization ($E_k = 0$), given by

$$n_o = \left[\frac{U_p + E_B}{w} \right] \tag{2.86}$$

The square bracket in Eq. (2.86) signifies the smallest integer containing the quantity within the bracket. The Fourier components f_n are given by

$$f_n = \frac{w}{2\pi} \int_0^{\frac{2\pi}{w}} dt e^{\iota(S(\vec{k}, t) - E_k t + nwt - U_p t)} \tag{2.87}$$

Now, if we set

$$T(n) = -\langle \vec{k} | \phi_i \rangle (E_k + E_B) f_n \tag{2.88}$$

then Eq. (2.85) can be written as

$$(S - 1)_{\text{fi}} = -2\pi\iota \sum_{n=n_o}^{\infty} \delta(E_k + E_B + U_p - nw) T(n) \tag{2.89}$$

The ionization probability per unit time \bar{w} is found from

$$\bar{w} = \lim_{t \rightarrow \infty} \frac{|(S - 1)_{\text{fi}}|^2}{t} \tag{2.90}$$

since,

$$\begin{aligned}
 2\pi\delta(E_k + E_B + U_p - mw)\delta(E_k + E_B + U_p - nw) &= \delta(E_k + E_B + U_p - nw) \\
 &\times \lim_{t \rightarrow \infty} \int_{-\frac{t}{2}}^{\frac{t}{2}} d\tau e^{\iota(E_k + E_B + U_p - mw)\tau} \\
 &= \delta(E_k + E_B + U_p - nw) \\
 &\times \lim_{t \rightarrow \infty} \int_{-\frac{t}{2}}^{\frac{t}{2}} d\tau e^{\iota(n-m)w\tau} \\
 &= \delta(E_k + E_B + U_p - nw) \\
 &\times \lim_{t \rightarrow \infty} \left[\frac{\sin \frac{1}{2}(n-m)wt}{\frac{1}{2}(n-m)w} \right]
 \end{aligned}$$

and

$$\lim_{t \rightarrow \infty} \frac{1}{t} \left[\frac{\sin \frac{1}{2}(n-m)wt}{\frac{1}{2}(n-m)w} \right] = \delta_{n,m}$$

and using Eq. (2.89) we obtain,

$$\bar{w} = 2\pi \sum_{n=n_0}^{\infty} \delta(E_k + E_B + U_p - nw) |T(n)|^2 \quad (2.91)$$

The total rate of ionization is found from integrating \bar{w} over all final states available to the ionized electron. The total ionization rate \bar{W} is thus

$$\begin{aligned} \bar{W} &= \int d\vec{k} \bar{w} \\ &= \int k^2 dk d\Omega \bar{w} \\ &= \int k dE_k d\Omega \bar{w} \end{aligned} \quad (2.92)$$

and therefore the differential ionization rate per unit energy, $w_{\text{fi}}(n, \theta)$ for the absorption of n photons with a momentum \vec{k} making an angle θ with a fixed z axis in space is given by

$$w_{\text{fi}}(n, \theta) = \frac{\partial^2 \bar{W}}{\partial E_k \partial \Omega} = k \bar{w} \quad (2.93)$$

Substituting Eq. (2.91) into Eq. (2.93) yields

$$w_{\text{fi}}(n, \theta) = 2\pi k(n) |T(n)|^2 \quad (2.94)$$

where the Fourier components are given by Eq. (2.87) and $k(n) = (2E_k)^{\frac{1}{2}}$ satisfies the energy conserving condition

$$E_k = nw - U_p - E_B$$

2.4.1 Ionization by Circularly Polarized Electromagnetic Field

We will consider now the case of a monochromatic circularly polarized electromagnetic plane wave. It is presumed that the electromagnetic field is adiabatically turned off at asymptotic times. The vector potential in dipole approximation (long wavelength approximation) for a plane wave propagating along the z axis is

$$\vec{A}(t) = \frac{A_0}{\sqrt{2}} (\cos wt \hat{x} \pm \sin wt \hat{y}) \quad (2.95)$$

where the upper (+) and lower (−) signs refer to right and left polarization, respectively. The semiclassical action for a free electron in the presence of such a wave is

$$\begin{aligned}
 S(\vec{k}, t) &= \frac{1}{2} \int^t d\tau (\vec{k} + \frac{1}{c} \vec{A})^2 \\
 &= E_k + \frac{A_0^2}{4c^2} + \frac{A_0}{2wc} k \sin \theta \sin(\omega t \mp \varphi) \\
 &= \frac{\sqrt{2U_p}}{w} k \sin \theta \sin(\omega t \mp \varphi) + E_k t + U_p t
 \end{aligned} \tag{2.96}$$

where $\vec{k} = (k, \theta, \varphi)$ is the electron momentum in spherical polar coordinates, in which the z axis is taken along the direction of propagation and U_p is the ponderomotive energy. The azimuthal angle φ and the ponderomotive energy U_p are given by,

$$\varphi = \arctan \frac{k_y}{k_x} \tag{2.97}$$

$$U_p = \frac{A_0^2}{4c^2} \tag{2.98}$$

The Fourier components f_n given by Eq. (2.87) now read

$$\begin{aligned}
 f_n &= \frac{w}{2\pi} \int_0^{\frac{2\pi}{w}} dt e^{i(S(\vec{k}, t) - E_k t - U_p t)} \\
 &= \frac{1}{2\pi} \int_0^{2\pi} d\vartheta e^{i(\frac{\sqrt{2U_p}}{w} k \sin \theta \sin(\vartheta \mp \varphi) + n\vartheta)}
 \end{aligned} \tag{2.99}$$

where we set $\vartheta = \omega t$. The use of the generating function for the Bessel function

$$\exp[i(\frac{\sqrt{2U_p}}{w} k \sin \theta \sin(\vartheta \mp \varphi))] = \sum_{m=-\infty}^{\infty} J_m(\frac{\sqrt{2U_p}}{w} k \sin \theta) e^{im(\vartheta \mp \varphi)} \tag{2.100}$$

and

$$\frac{1}{2\pi} \int_0^{2\pi} d\vartheta e^{i(m+n)\vartheta} = \delta_{m, -n}$$

puts the the integral for f_n in closed analytical form

$$\begin{aligned}
 f_n &= J_{-n}(\frac{\sqrt{2U_p}}{w} k \sin \theta) e^{\pm in\varphi} \\
 &= (-1)^n J_n(\frac{\sqrt{2U_p}}{w} k \sin \theta) e^{\pm in\varphi}
 \end{aligned} \tag{2.101}$$

From Eq. (2.88) we get for $T(n)$

$$T(n) = -\langle \vec{k} | \phi_i \rangle (E_k + E_B) (-1)^n J_n(\frac{\sqrt{2U_p}}{w} k \sin \theta) e^{\pm in\varphi} \tag{2.102}$$

Finally from Eq. (2.93) we arrive at the differential ionization rate, $w_{\text{fi}}(n, \theta)$, for the absorption of n photons with a momentum \vec{k} making an angle θ with the direction of propagation of the circularly polarized electromagnetic field

$$w_{\text{fi}}(n, \theta) = 2\pi k(n) |\langle \vec{k} | \phi_i \rangle|^2 |(E_k + E_B)|^2 |J_n(\frac{\sqrt{2U_p}}{w} k \sin \theta)|^2 \quad (2.103)$$

with the conservation of energy condition

$$E_k = \frac{k(n)^2}{2} = (nw - E_B - U_p) \quad (2.104)$$

By examining Eq. (2.103) it is easy to see, since $J_n(0) = \delta_{n,0}$ and $n \geq n_o = [\frac{U_p + E_B}{w}]$, that no electrons can be detected along the direction of propagation or with threshold energy; i.e., $E_k \approx 0$, and those that are detected are peaked in the polarization plane. This is due to angular momentum conservation considerations. Due to conservation of angular momentum, the absorption of n photons in the ionization of an electron by circularly polarized field, demands the transfer of n units of angular momentum to the ionized electron, thus prohibiting the detection of electrons along the direction of propagation or with zero energy and peaking in the polarization plane. Moreover, electrons are peaked in the polarization plane with energy equaling the ponderomotive energy, in agreement with the classical model presented in the previous chapter.

2.4.2 Ionization by Linearly Polarized Electromagnetic Field

The vector potential for a monochromatic linearly polarized plane wave in the long wavelength approximation is

$$\vec{A}(t) = A_0 \hat{e} \cos wt \quad (2.105)$$

where \hat{e} is a unit vector. Introducing $\vec{\alpha}(t)$

$$\vec{\alpha}(t) = \frac{1}{c} \int^t d\tau \vec{A}(\tau) = \frac{2\sqrt{U_p}}{w} \hat{e} \sin wt \quad (2.106)$$

The semiclassical action for a free electron in such a wave is

$$\begin{aligned} S(\vec{k}, t) &= \frac{1}{2} \int^t d\tau (\vec{k} + \frac{1}{c} \vec{A})^2 \\ &= E_k t + U(t) + \vec{k} \cdot \vec{\alpha}(t) \end{aligned} \quad (2.107)$$

with

$$\begin{aligned} U(t) &= \frac{1}{2c^2} \int^t d\tau A^2(\tau) = U_p t + U_1(t) \\ U_1 &= \frac{U_p}{2w} \sin 2wt \\ U_p &= \frac{A_0^2}{4c^2} \end{aligned}$$

The Fourier components given by Eq. (2.87) now read

$$\begin{aligned} f_n &= \frac{w}{2\pi} \int_0^{2\pi} dt e^{i(\frac{2\sqrt{U_p}}{w} \vec{k} \cdot \vec{\epsilon} \sin wt + \frac{U_p}{2w} \sin 2wt + nwt)} \\ &= \frac{1}{2\pi} \int_0^{2\pi} d\vartheta e^{i(\frac{2\sqrt{U_p}}{w} k \cos \theta \sin \vartheta + \frac{U_p}{2w} \sin 2\vartheta + n\vartheta)} \\ &= \frac{(-1)^n}{2\pi} \int_{-\pi}^{\pi} d\vartheta e^{i(\frac{2\sqrt{U_p}}{w} k \cos \theta \sin \vartheta - \frac{U_p}{2w} \sin 2\vartheta - n\vartheta)} \end{aligned} \quad (2.108)$$

where we set $\vartheta = wt$ and $\vec{k} = (k, \theta, \varphi)$ is the electron momentum in spherical polar coordinates, in which the z axis is taken along the direction of polarization $\vec{\epsilon}$. The use of the generalized Bessel function definition [26]

$$J_n(x, y) = \frac{1}{2\pi} \int_{-\pi}^{\pi} d\vartheta e^{i(x \sin \vartheta + y \sin 2\vartheta - n\vartheta)} \quad (2.109)$$

puts the integral for f_n in closed analytical form

$$\begin{aligned} f_n &= (-1)^n J_{-n}\left(\frac{2\sqrt{U_p}}{w} k \cos \theta, -\frac{U_p}{2w}\right) \\ &= J_n\left(\frac{2\sqrt{U_p}}{w} k \cos \theta, -\frac{U_p}{2w}\right) \end{aligned} \quad (2.110)$$

From Eq. (2.88) we get for $T(n)$

$$T(n) = -\langle \vec{k} | \phi_i \rangle (E_k + E_B) J_n\left(\frac{2\sqrt{U_p}}{w} k \cos \theta, -\frac{U_p}{2w}\right) \quad (2.111)$$

Finally from Eq. (2.93) we arrive at the differential ionization rate $w_{\text{fi}}(n, \theta)$ for the absorption of n photons with a momentum \vec{k} making an angle θ with the direction of polarization of the linearly polarized electromagnetic field

$$w_{\text{fi}}(n, \theta) = 2\pi k(n) |\langle \vec{k} | \phi_i \rangle|^2 (E_k + E_B)^2 |J_n\left(\frac{2\sqrt{U_p}}{w} k \cos \theta, -\frac{U_p}{2w}\right)|^2 \quad (2.112)$$

with the conservation of energy condition

$$E_k = \frac{k(n)^2}{2} = (nw - E_B - U_p) \quad (2.113)$$

Examining Eq. (2.12) it is easy to see, unlike the circularly polarized case, ionized electrons peak in the forward direction around the threshold energy ($E_k \approx 0$) up to $2U_p$, in agreement with the classical model discussed in the previous chapter. Here, no net units of angular momenta are transferred in the ionization process.

Chapter 3

Theory II

The KFR theory presented in chapter 2 ignores the residual Coulomb effects in the dynamics of the the final state of the complete system of an atom in the presence of strong electromagnetic field. When $\frac{U_P}{E_B} \gg 1$, then the subsequent dynamics of the free electron is dominated by the strong electromagnetic field, where it will propagate in the strong electromagnetic until it exits the field and arrives at a detector. These electrons suffer no interaction with the parent ions and are therefore called *direct electrons*. However, the experimental findings[8-13] of the high energy part of the ATI spectrum and the high harmonics generation (HHG), necessitate the consideration of rescattering. Here electrons interact with the parent ions and re-scatter before exiting the electromagnetic field and then arrive at a detector. In this chapter we will develop a theoretical formulation for the quantum mechanical consideration of rescattering.

Within the single active electron model, the dynamics of an atom in the presence of strong electromagnetic field is described by the Schrödinger equation

$$(i\frac{\partial}{\partial t} - H_0 - V_A - V_L)\Psi = 0 \quad (3.1)$$

where $H_0 = -\frac{\nabla^2}{2}$ is the kinetic energy Hamiltonian operator for a free particle, V_A is the atomic binding potential and V_L is the laser-atom interaction Hamiltonian, which in the

velocity gauge is given by

$$V_L(t) = \frac{1}{c} \vec{A} \cdot (-i\vec{\nabla}) + \frac{A^2}{2c^2} \quad (3.2)$$

Our starting point is Eq. (2.59), which is the *time reverse* exact expression for the S matrix

$$(S - 1)_{\text{fi}} = -i \int_{-\infty}^{\infty} dt \langle \Psi_{\text{f}}^{(-)} | V_L \phi_{\text{i}} \rangle \quad (3.3)$$

3.1 Difficulty in an *ab initio* Formulation of Rescattering

Initially, on first principles, we will develop an *ab initio* consideration of rescattering where the long-range Coulomb effects are taken into account in the dynamics of the final state of the complete system. As we will see, this results in a singular S matrix and consequently a regularization of the resulting S matrix is required.

To this effect, using Eq. (2.54), we write for the final state wave function $\Psi_{\text{f}}^{(-)}(t)$

$$\Psi_{\text{f}}^{(-)}(t) = \Psi_{\vec{k}}^{(\text{v})} + \int_t^{\infty} dt' G_{\text{L}}^{(-)}(t, t') V_{\text{A}}(t') \Psi_{\text{f}}^{(-)}(t') \quad (3.4)$$

where $\Psi_{\vec{k}}^{(\text{v})}$ is a Volkov state, and $G_{\text{L}}^{(+)}$ is the Volkov propagator. Next, within the SFA, we replace $\Psi_{\text{f}}^{(-)}$ in the right hand side of Eq. (3.4) by $\Psi_{\vec{k}}^{(\text{v})}$ thus we obtain

$$\Psi_{\text{f}}^{(-)}(t) \approx \Psi_{\vec{k}}^{(\text{v})} + \int_t^{\infty} dt' G_{\text{L}}^{(-)}(t, t') V_{\text{A}}(t') \Psi_{\vec{k}}^{(\text{v})}(t') \quad (3.5)$$

Substituting for $\Psi_{\text{f}}^{(-)}$ in Eq. (3.3) and using $G_{\text{L}}^{(-)\dagger}(t, t') = G_{\text{L}}^{(+)}(t', t)$, we obtain

$$(S-1)_{\text{fi}} \approx -i \int_{-\infty}^{\infty} dt \langle \Psi_{\vec{k}}^{(\text{v})}(t) | V_{\text{L}}(t) \phi_{\text{i}}(t) \rangle - i \int_{-\infty}^{\infty} dt \int_{-\infty}^t dt' \langle \Psi_{\vec{k}}^{(\text{v})}(t) | V_{\text{A}} G_{\text{L}}^{(+)}(t, t') V_{\text{L}}(t') \phi_{\text{i}}(t') \rangle \quad (3.6)$$

The first term on the right hand side of Eq. (3.6) is the KFR direct electron term and we will denote it by $S_{\text{fi}}^{(0)}$

$$S_{\text{fi}}^{(0)} = -i \int_{-\infty}^{\infty} dt \langle \Psi_{\vec{k}}^{(\text{v})}(t) | V_{\text{L}}(t) \phi_{\text{i}}(t) \rangle \quad (3.7)$$

and the second term is the rescattered electrons term and we will denote it by $S_{\text{fi}}^{(1)}$

$$S_{\text{fi}}^{(1)} = -i \int_{-\infty}^{\infty} dt \int_{-\infty}^t dt' \langle \Psi_{\vec{k}}^{(\text{v})}(t) | V_{\text{A}} G_{\text{L}}^{(+)}(t, t') V_{\text{L}}(t') \phi_{\text{i}}(t') \rangle \quad (3.8)$$

therefore Eq. (3.6) is rewritten as

$$(S - 1)_{\text{fi}} \approx S_{\text{fi}}^{(0)} + S_{\text{fi}}^{(1)} \quad (3.9)$$

The physical interpretation of of Eqs. (3.6)-(3.9) is as follows. Due to the interaction with the laser field, the electron gets ionized from the initial ground state. After that, the electron propagates in the laser field and it also feels the long-range Coulomb field. It can then leave these fields and can be observed experimentally and this corresponds to the term $S_{\text{fi}}^{(0)}$. It can, however, happen that during this propagation the ionized electron comes back to atomic core and rescatters due to the short range part of the atomic potential and this corresponds to the term $S_{\text{fi}}^{(1)}$. After rescattering the electron propagates out of the fields and can be observed. Of course, both contributions interfere quantum mechanically as shown in Eq. (3.9).

To evaluate $S_{\text{fi}}^{(1)}$, we use Eq. (2.49) to write the Volkov propagator as

$$G_{\text{L}}^{(+)}(t, t') = -i\Theta(t - t') \int d\vec{q} | \Psi_{\vec{q}}^{(\text{v})}(t) \rangle \langle \Psi_{\vec{q}}^{(\text{v})}(t') | e^{-\eta(t-t')} \quad (3.10)$$

where, $\eta \rightarrow 0^+$ is implied by the outgoing boundary conditions. Substituting for $G_{\text{L}}^{(+)}$ in Eq. (3.8) gives

$$\begin{aligned} S_{\text{fi}}^{(1)} &= -i \int d\vec{q} \int_{-\infty}^{\infty} dt \int_{-\infty}^t dt' \langle \Psi_{\vec{k}}^{(\text{v})}(t) | V_{\text{A}} | \Psi_{\vec{q}}^{(\text{v})}(t) \rangle (-i) \langle \Psi_{\vec{q}}^{(\text{v})}(t') | V_{\text{L}}(t') \phi_{\text{i}}(t') \rangle e^{-\eta(t-t')} \\ &= -i \int d\vec{q} \int_{-\infty}^{\infty} dt \langle \Psi_{\vec{k}}^{(\text{v})}(t) | V_{\text{A}} | \Psi_{\vec{q}}^{(\text{v})}(t) \rangle (-i) \int_{-\infty}^t dt' \langle \Psi_{\vec{q}}^{(\text{v})}(t') | V_{\text{L}}(t') \phi_{\text{i}}(t') \rangle e^{-\eta(t-t')} \end{aligned} \quad (3.11)$$

Just as the amplitude $S_{\text{fi}}^{(0)}$ of the direct ATI process has a simple physical interpretation in which, after initial absorption of incident field photons and release from the initial ground state ϕ_{i} , the released electron escapes eventually to final continuum state $\Psi_{\vec{k}}^{(\text{v})}$ with canonical momentum \vec{k} corresponding to lower energy photoelectrons, the expression (3.11) for the rescattering ATI amplitude, $S_{\text{fi}}^{(1)}$, allows for a quite transparent physical interpretation. The structure of Eq. (3.11) signifies the continuum-continuum transitions role in the production of the high energy photoelectrons. After initial absorption of incident field photons, caused by the laser-atom interaction operator V_{L} , the initially bound electron is

released from the ground state ϕ_i into intermediate continuum state $\Psi_{\vec{q}}^{(v)}$, with canonical momentum \vec{q} . Afterwards, being still in the neighborhood of the parent core and driven further by the laser field into the vicinity of the atomic core, the ionized electron rescatters off the parent atomic core due to the interaction operator V_A with a scattering atomic potential. During the course of the rescattering process, the released electron undergoes a considerable acceleration, making a transition from an intermediate continuum state with canonical momentum \vec{q} into a final continuum state with canonical momentum \vec{k} . Owing to this process (inverse bremsstrahlung), the released electron is able to absorb an additional number of extra photons and escape eventually with higher energy than would be possible without this process. This explains the origin of the high energy plateau of the ATI spectrum.

Now let us define $\Gamma(t)$ to be the transition amplitude from initial ground state ϕ_i into a intermediate continuum state $\Psi_{\vec{q}}^{(v)}$ at time t

$$\Gamma(t) = (-i) \int_{-\infty}^t dt' \langle \Psi_{\vec{q}}^{(v)}(t') | V_L(t') \phi_i(t') \rangle e^{-\eta(t-t')} \quad (3.12)$$

where the initial ground state ϕ_i and the Volkov state $\Psi_{\vec{q}}^{(v)}$ are given by (see Eqs. (2.80) and (2.77))

$$\begin{aligned} |\phi_i(\vec{r}, t')\rangle &= |\phi_i(\vec{r})\rangle e^{-iE_i t'} \\ |\Psi_{\vec{q}}^{(v)}(t')\rangle &= e^{-iS(\vec{q}, t')} |\vec{q}\rangle \end{aligned}$$

If we set $t = +\infty$, then Γ becomes $S_{\text{fi}}^{(0)}$ with \vec{k} is replaced with \vec{q} . Proceeding, as we did in Ch. (2), in the evaluation of $S_{\text{fi}}^{(0)}$ we arrive at

$$\begin{aligned} \Gamma &= -i \langle \vec{q} | \phi_i(\vec{r}) \rangle \int_{-\infty}^t dt' e^{i(\frac{q^2}{2} - E_i)t'} V_L(\vec{q}, t') e^{i \int_{-\infty}^{t'} dt'' V_L(\vec{q}, t'')} e^{-\eta(t-t')} \\ &= -i \langle \vec{q} | \phi_i(\vec{r}) \rangle \int_{-\infty}^t dt' e^{iS(\vec{q}, t')} \left(\dot{S}(\vec{q}, t') - \frac{q^2}{2} \right) e^{-iE_i t'} e^{-\eta(t-t')} \end{aligned} \quad (3.13)$$

Carrying out integration by parts over t' we obtain

$$\begin{aligned} \Gamma &= -\langle \vec{q} | \phi_i(\vec{r}) \rangle \left\{ e^{iS(\vec{q}, t)} e^{-iE_i} \right. \\ &\quad \left. - i(E_q - E_i - \eta) \int_{-\infty}^t dt' e^{i(S(\vec{q}, t') - E_q t' - U_p t')} e^{i(E_q - E_i + U_p)t'} e^{-\eta(t-t')} \right\} \end{aligned} \quad (3.14)$$

$S(\vec{q}, t') - E_q t' - U_p t'$ is periodic in t' with period equals $\frac{2\pi}{w}$, so we write (see Eq. (2.84))

$$e^{i(S(\vec{q}, t') - E_q t' - U_p t')} = \sum_{n=-\infty}^{\infty} f_n e^{-inwt'} \quad (3.15)$$

substituting Eq. (3.15) into Eq. (3.14) we obtain

$$\begin{aligned} \Gamma &= -\langle \vec{q} | \phi_i(\vec{r}) \rangle \left\{ \sum_{n=-\infty}^{\infty} f_n e^{i(E_q - E_i + U_p - nw)t} \right. \\ &\quad \left. - \sum_{n=-\infty}^{\infty} f_n e^{i(E_q - E_i + U_p - nw)t} \frac{E_q - E_i - \eta}{E_q - E_i + U_p - nw - \eta} \right\} \\ &= -\langle \vec{q} | \phi_i(\vec{r}) \rangle \sum_{n=-\infty}^{\infty} f_n \frac{(U_p - nw)}{E_q - E_i + U_p - nw - \eta} e^{i(E_q - E_i + U_p - nw)t} \end{aligned} \quad (3.16)$$

Substituting Eq. (3.16) for Γ into Eq. (3.11) we obtain for $S_{\text{fi}}^{(1)}$ the following expression

$$\begin{aligned} S_{\text{fi}}^{(1)} &= i \int d\vec{q} \langle \vec{q} | \phi_i(\vec{r}) \rangle \langle \vec{k} | V_A | \vec{q} \rangle \int_{-\infty}^{\infty} dt e^{i(S(\vec{k}, t) - S(\vec{q}, t))} \\ &\quad \times \sum_{n=-\infty}^{\infty} f_n \frac{(U_p - nw)}{E_q - E_i + U_p - nw - \eta} e^{i(E_q - E_i + U_p - nw)t} \end{aligned} \quad (3.17)$$

Since

$$\begin{aligned} e^{i(S(\vec{k}, t) - S(\vec{q}, t))} &= e^{i(E_k - E_q + (\vec{k} - \vec{q}) \cdot \vec{\alpha})} \\ &= \sum_{m=-\infty}^{\infty} g_m e^{i(E_k - E_i - mw)t} \end{aligned} \quad (3.18)$$

where $\vec{\alpha}$ and the Fourier components g_m are given by

$$\vec{\alpha} = \frac{1}{c} \int_{-\infty}^t d\tau A(\vec{\tau}) \quad (3.19)$$

$$g_m = \frac{w}{2\pi} \int_0^{\frac{2\pi}{w}} dt e^{i(\vec{k} - \vec{q}) \cdot \vec{\alpha}} e^{imwt} \quad (3.20)$$

then Eq. (3.17) reads

$$\begin{aligned} S_{\text{fi}}^{(1)} &= i \int d\vec{q} \langle \vec{q} | \phi_i(\vec{r}) \rangle \langle \vec{k} | V_A | \vec{q} \rangle \int_{-\infty}^{\infty} dt \\ &\quad \times \sum_{n=-\infty}^{\infty} \sum_{m=-\infty}^{\infty} f_n g_m \frac{(U_p - nw)}{E_q - E_i + U_p - nw - \eta} \\ &\quad \times e^{i(E_k - E_i + U_p - (n+m)w)t} \end{aligned} \quad (3.21)$$

Letting the dummy index $n \rightarrow m - n$ and carrying out the trivial integral over t we obtain

$$S_{\text{fi}}^{(1)} = 2\pi\iota \sum_{m=n_0}^{\infty} \delta(E_k + E_B + U_p - mw) \int d\vec{q} \langle \vec{q} | \phi_i(\vec{r}) \rangle \langle \vec{k} | V_A | \vec{q} \rangle \\ \times \sum_{n=n_0}^{\infty} \frac{U_p - nw}{E_q + E_B + U_p - nw - i\eta} f_n g_{m-n} \quad (3.22)$$

interchanging the dummy indices n and m and setting $E_B = -E_i$ we finally obtain

$$S_{\text{fi}}^{(1)} = 2\pi\iota \sum_{n=n_0}^{\infty} \delta(E_k + E_B + U_p - nw) \int d\vec{q} \langle \vec{q} | \phi_i(\vec{r}) \rangle \langle \vec{k} | V_A | \vec{q} \rangle \\ \times \sum_{m=n_0}^{\infty} \frac{U_p - mw}{E_q + E_B + U_p - mw - i\eta} f_m g_{n-m} \quad (3.23)$$

For a Coulomb like atomic binding potential $V_A = -\frac{Z}{r}$, where Z is the effective charge of atomic core, we have

$$\langle \vec{k} | V_A | \vec{q} \rangle = -\frac{Z}{2\pi^2 |\vec{k} - \vec{q}|^2} \quad (3.24)$$

and therefore, in the limit $\eta \rightarrow 0^+$, it is clear that for $m = n$ the integrand in Eq. (3.23) is singular and so is $S_{\text{fi}}^{(1)}$. When $m \neq n$, the integrand has simple poles corresponding to resonances representing the essential continuum state channels responsible for continuum-continuum transitions. To overcome this setback, we could use for V_A a short range screened Yukawa type potential $V_A = -\frac{Z e^{-\lambda r}}{r}$ and so we have

$$\langle \vec{k} | V_A | \vec{q} \rangle = -\frac{Z}{2\pi^2 |\vec{k} - \vec{q}|^2 + \lambda^2} \quad (3.25)$$

and therefore the integrand has only simple poles. However we will proceed on first principles and devise a scheme to regularize the singularity.

3.1.1 Regularization of Singularity

To this end, we will split $S_{\text{fi}}^{(1)}$ into a regular part $S_{\text{r}}^{(1)}$ and irregular (singular) part $S_{\text{ir}}^{(1)}$ so that

$$S_{\text{fi}}^{(1)} = S_{\text{r}}^{(1)} + S_{\text{ir}}^{(1)} \quad (3.26)$$

with

$$S_{\text{r}}^{(1)} = 2\pi\iota \sum_{n=n_0}^{\infty} \delta(E_k + E_B + U_p - nw) \int d\vec{q} \langle \vec{q} | \phi_i(\vec{r}) \rangle \langle \vec{k} | V_A | \vec{q} \rangle$$

$$\times \sum_{m=n_0}^{\infty'} \frac{U_p - mw}{E_q + E_B + U_p - mw - i\eta} f_m g_{n-m} \quad (3.27)$$

where, \sum' indicates the term $m = n$ is excluded from the sum, and

$$\begin{aligned} S_{\text{ir}}^{(1)} &= 2\pi i \sum_{n=n_0}^{\infty} \delta(E_k + E_B + U_p - nw) \int d\vec{q} \langle \vec{q} | \phi_i(\vec{r}) \rangle \langle \vec{k} | V_A | \vec{q} \rangle \\ &\times \frac{U_p - nw}{E_q + E_B + U_p - nw - i\eta} f_n g_0 \end{aligned} \quad (3.28)$$

The $m = n$ term, i.e. $S_{\text{ir}}^{(1)}$, has a simple physical interpretation. n is the number of absorbed photons for ionization from the initial state to intermediate continuum states with canonical momentum \vec{q} to the final continuum states with canonical momentum \vec{k} and m is the number of absorbed photons for ionization from the initial state to intermediate states with canonical momentum \vec{q} . Then $m = n$ means that the transitions from intermediate continuum states to final continuum states are associated with no emission or absorption of extra photons. This happens when the initially bound electron is promoted into the intermediate continuum state near the end of duration of laser pulse and consequently it will scatter off the atomic core from the intermediate canonical momentum \vec{q} into final canonical momentum \vec{k} . Therefore this term does not contribute to the high energy plateau of the ATI spectrum; rather it does contribute to the low energy direct electrons. Only S_{r}^1 is relevant to the high energy electrons of the ATI spectrum and this has a significant physical implication.

In the laboratory frame, the atom is sitting in an oscillating electromagnetic field. If we go to a frame that oscillates in phase with the electromagnetic field, then the electron sees an oscillating nucleus. In this frame the ionized electron scatters off an oscillating Coulomb center. Consequently, in this frame, the regular nonsingular part of the the wave function, which is relevant for the production of high energy electrons, is identified as well as the singular part, which contributes to the low energy direct electrons. This identification enables the regularization of the wave function. The transformation from the laboratory frame to the oscillating frame is achieved through a unitary transformation called the Henneberger transformation [70].

Thus we introduce a new wave function $\Phi_{\mathbf{f}}^{(-)}$

$$\Psi_{\mathbf{f}}^{(-)} = e^{-i \int^t d\tau V_L(\tau)} \Phi_{\mathbf{f}}^{(-)} \quad (3.29)$$

then the Schrödinger equation, Eq. (3.1), reads

$$(i \frac{\partial}{\partial t} - H_o - e^{i\alpha \cdot \vec{p}} V_A e^{-i\alpha \cdot \vec{p}}) \Phi_{\mathbf{f}}^{(-)} = 0 \quad (3.30)$$

where $\vec{\alpha}$ is given by Eq. (3.19). Since

$$e^{i\alpha \cdot \vec{p}} V_A e^{-i\alpha \cdot \vec{p}} = V_A(\vec{r} + \vec{\alpha}) \quad (3.31)$$

then we obtain

$$(i \frac{\partial}{\partial t} - H_o - V_A(\vec{r} + \vec{\alpha})) \Phi_{\mathbf{f}}^{(-)} = 0 \quad (3.32)$$

To first order in $V_A(\vec{r} + \vec{\alpha})$, using Dirac bra-ket notation, we have (see Eq. (2.54))

$$| \Phi_{\mathbf{f}}^{(-)}(t) \rangle \approx | \chi_{\vec{k}}^{(-)}(t) \rangle + \int_t^\infty dt' G_o^{(-)}(t, t') V_A(\vec{r} + \vec{\alpha}(t')) | \chi_{\vec{k}}^{(-)}(t') \rangle \quad (3.33)$$

where $\chi_{\vec{k}}^{(-)}(t) = \langle \vec{r} | \vec{k} \rangle e^{-iE_k t}$ is a plane wave. The singularity in $S_{\text{ir}}^{(1)}$, i.e. $S_{\text{ir}}^{(1)}$, comes from the singularity in $| \Phi_{\mathbf{f}}^{(-)} \rangle$ and this happen when $\vec{\alpha} = 0$ (i.e. when the laboratory frame and the Henneberger frame coincides). To see this, we write Eq. (3.33) as

$$| \Phi_{\mathbf{f}}^{(-)}(t) \rangle \approx | \Phi_{\mathbf{f}}^{(0)}(t) \rangle + | \Phi_{\mathbf{f}}^{(1)}(t) \rangle \quad (3.34)$$

with

$$| \Phi_{\mathbf{f}}^{(0)}(t) \rangle = | \chi_{\vec{k}}^{(-)}(t) \rangle = | \vec{k} \rangle e^{-iE_k t} \quad (3.35)$$

$$| \Phi_{\mathbf{f}}^{(1)}(t) \rangle = \int_t^\infty dt' G_o^{(-)}(t, t') V_A(\vec{r} + \vec{\alpha}(t')) | \chi_{\vec{k}}^{(-)}(t') \rangle \quad (3.36)$$

The advanced free particle propagator $G^{(-)}(t, t')$ is given by

$$G^{(-)}(t, t') = i \Theta(t', t) \int d\vec{q} | \vec{q} \rangle \langle \vec{q} | e^{-iE_q(t-t')} e^{-\eta(t-t')} \quad (3.37)$$

where, $\eta \rightarrow 0^-$ is implied by incoming boundary conditions.

Let $\Phi_{\text{ir}}^{(1)}$ be the wave function $\Phi_{\mathbf{f}}^{(1)}$ when $\vec{\alpha} = 0$. From Eq. (3.36) $\Phi_{\text{ir}}^{(1)}$ is

$$| \Phi_{\text{ir}}^{(1)}(t) \rangle = \int_t^\infty dt' G_o^{(-)}(t, t') V_A(\vec{r}) | \chi_{\vec{k}}^{(-)}(t') \rangle \quad (3.38)$$

Substituting Eq. (3.37) into Eq. (3.38) we obtain

$$\begin{aligned}\Phi_{\text{ir}}^{(1)}(\vec{r}, t) &= \langle \vec{r} | \Phi_{\text{ir}}^{(1)}(t) \rangle = \imath \int_t^\infty dt' \int d\vec{q} e^{-\imath E_q t} \langle \vec{r} | \vec{q} \rangle \langle \vec{q} | V_A | \vec{k} \rangle \\ &\times e^{-\imath(E_k - E_q)t'} e^{-\eta(t-t')} \end{aligned} \quad (3.39)$$

$$= \imath \frac{-4\pi Z}{(2\pi)^{\frac{3}{2}}} \int d\vec{q} \frac{e^{\imath\vec{q}\cdot\vec{r}}}{|\vec{q} - \vec{k}|^2} e^{-\imath(E_q - \imath\eta)t} \int_t^\infty dt' e^{-\imath(E_k - E_q + \imath\eta)t'} \quad (3.40)$$

where we have used Eq. (3.24) and $\langle \vec{r} | \vec{q} \rangle = \frac{1}{(2\pi)^{\frac{3}{2}}} e^{\imath\vec{q}\cdot\vec{r}}$ and it is understood that $\eta \rightarrow 0^-$.

The integral over t' is trivial and we obtain

$$\Phi_{\text{ir}}^{(1)}(\vec{r}, t) = \frac{4\pi Z}{(2\pi)^{\frac{3}{2}}} e^{-\imath E_k t} \int d\vec{q} \frac{e^{\imath\vec{q}\cdot\vec{r}}}{|\vec{q} - \vec{k}|^2 (E_q - E_k - \imath\eta)} \quad (3.41)$$

Setting $E_k = \frac{k^2}{2}$ and $E_q = \frac{q^2}{2}$ and using Feynmann two denominator integral formula [89]

$$\frac{1}{|\vec{q} - \vec{k}|^2 (q^2 - k^2 - 2\imath\eta)} = \int_0^1 \frac{dx}{\{[q^2 - k^2 - 2\imath\eta]x + [q^2 + k^2 - 2\vec{q}\cdot\vec{k}](1-x)\}^2} \quad (3.42)$$

so that

$$\Phi_{\text{ir}}^{(1)}(\vec{r}, t) = \frac{8\pi Z}{(2\pi)^{\frac{3}{2}}} e^{-\imath E_k t} \int_0^1 dx e^{\imath(1-x)\vec{k}\cdot\vec{r}} \int d\vec{p} \frac{e^{\imath\vec{p}\cdot\vec{r}}}{[p^2 - \beta^2]^2} \quad (3.43)$$

with

$$\begin{aligned}\vec{p} &= \vec{q} - (1-x)\vec{k} \\ \beta^2 &= x(xk^2 + 2\imath\eta)\end{aligned}$$

By choosing the z -axis in the \vec{p} direction then the integral over the angles is straightforward and the remaining integral over p is evaluated using techniques of complex variables theory so that

$$\begin{aligned}\Phi_{\text{ir}}^{(1)}(\vec{r}, t) &= \imath \frac{8(\pi)^3 Z}{(2\pi)^{\frac{3}{2}}} e^{-\imath E_k t} \int_0^1 dx e^{\imath(1-x)\vec{k}\cdot\vec{r}} \frac{e^{\imath\sqrt{x(xk^2+2\imath\eta)}r}}{\sqrt{x(xk^2+2\imath\eta)}} \\ &= \imath(2\pi)^{\frac{3}{2}} Z e^{[\imath\vec{k}\cdot\vec{r} - \imath E_k t]} \int_0^1 dx \frac{e^{[-\imath\vec{k}\cdot\vec{r}x + \imath\sqrt{x^2k^2+2\imath x\eta}r]}}{\sqrt{x^2k^2+2\imath x\eta}} \end{aligned} \quad (3.44)$$

$\Phi_{\text{ir}}^{(1)}$ as given by Eq. (3.44) has a logarithmic divergence in the limit $\eta \rightarrow 0$. To see this we write

$$\Phi_{\text{ir}}^{(1)} = \imath(2\pi)^{\frac{3}{2}} Z e^{[\imath\vec{k}\cdot\vec{r} - \imath E_k t]} \left\{ \int_0^1 dx \frac{e^{[-\imath\vec{k}\cdot\vec{r}x + \imath\sqrt{x^2k^2+2\imath x\eta}r]} - 1}{\sqrt{x^2k^2+2\imath x\eta}} + \int_0^1 \frac{dx}{\sqrt{x^2k^2+2\imath x\eta}} \right\} \quad (3.45)$$

The second integral on the right hand side of Eq. (3.45) is easily evaluated to be equal to $-\frac{1}{k} \ln(\frac{\eta}{2k^2})$.

Now we set

$$\iota(kr - \vec{k} \cdot \vec{r})x = y$$

so that for small η we have

$$\Phi_{\text{ir}}^{(1)} = \frac{\iota(2\pi)^{\frac{3}{2}} Z}{k} e^{[\iota\vec{k} \cdot \vec{r} - \iota E_k t]} \left\{ \int_0^{\iota(kr - \vec{k} \cdot \vec{r})} dy \frac{e^y - 1}{y} - \ln\left(\frac{\eta}{2k^2}\right) \right\} \quad (3.46)$$

The integral over y is identified as an integral representation of the exponential integral function $\text{Ei}(z)$ [71] and so we have

$$\Phi_{\text{ir}}^{(1)} = \frac{\iota(2\pi)^{\frac{3}{2}} Z}{k} e^{[\iota\vec{k} \cdot \vec{r} - \iota E_k t]} \left\{ \text{Ei}[\iota(kr - \vec{k} \cdot \vec{r})] - \ln[\iota(kr - \vec{k} \cdot \vec{r})] - \gamma - \ln\left(\frac{\eta}{2k^2}\right) \right\} \quad (3.47)$$

where γ is Euler's constant. It is obvious that $\Phi_{\text{ir}}^{(1)}$ has a logarithmic divergence as $\eta \rightarrow 0$. Later in this section we will show how to regularize $\Phi_{\text{ir}}^{(1)}$.

Next, we solve Eq. (3.36) when $\vec{\alpha} \neq 0$. Substituting Eq. (3.37) into Eq. (3.36) and setting $\tau = t - t'$ we obtain

$$\Phi_{\text{f}}^{(1)}(\vec{r}, t) = \iota \langle \vec{r} | \Phi_{\text{f}}^{(1)} \rangle = \int_t^\infty dt' \int d\vec{q} \int d\vec{r}' e^{\iota\vec{q} \cdot (\vec{r} - \vec{r}')} e^{-\iota E_q \tau} V_{\text{A}}(\vec{r}' + \vec{\alpha}(t')) e^{\iota\vec{k} \cdot \vec{r}'} e^{-\iota E_k t'} e^{-\eta\tau} \quad (3.48)$$

The integral over \vec{q} is straightforward yielding

$$\Phi_{\text{f}}^{(1)}(\vec{r}, t) = \langle \vec{r} | \Phi_{\text{f}}^{(1)} \rangle = \iota \int_t^\infty dt' \frac{1}{(2\pi\iota\tau)^{\frac{3}{2}}} \int d\vec{r}' e^{\iota[\frac{(\vec{r} - \vec{r}')^2}{2\tau} + \iota\vec{k} \cdot \vec{r}' - \iota E_k t']} V_{\text{A}}(\vec{r}' + \vec{\alpha}(t')) e^{-\eta\tau} \quad (3.49)$$

Now write

$$\frac{(\vec{r} - \vec{r}')^2}{2\tau} + \vec{k} \cdot \vec{r}' = \frac{(\vec{r}' - \vec{\rho}_0)^2}{2\tau} + \vec{k} \cdot \vec{r}' - E_k \tau$$

with

$$\vec{\rho}_0 = \vec{r} - \vec{k}\tau$$

and define

$$\begin{aligned} \vec{r}'' &= \vec{r}' - \vec{\rho}_0 \\ \vec{\rho} &= \vec{\alpha} + \vec{\rho}_0 \end{aligned}$$

then Eq. (3.39) reads

$$\Phi_f^{(1)}(\vec{r}, t) = \imath \int_t^\infty dt' \frac{1}{(2\pi\imath\tau)^{\frac{3}{2}}} e^{[\imath\vec{k}\cdot\vec{r}-\imath E_k\tau-\imath E_k t']} e^{-\eta\tau} \int d\vec{r}'' e^{\imath\frac{r''^2}{2\tau}} V_A(\vec{r}'' + \vec{\rho}) \quad (3.50)$$

For a hydrogenlike atomic core

$$V_A(\vec{r}'' + \vec{\rho}) = -\frac{Z}{|\vec{r}'' + \vec{\rho}|} \quad (3.51)$$

where Z is an effective atomic core charge. The integral over the angles is trivial and therefore we have

$$\Phi_f^{(1)}(\vec{r}, t) = \imath \int_t^\infty dt' \frac{-4\pi Z}{(2\pi\imath\tau)^{\frac{3}{2}}} e^{[\imath\vec{k}\cdot\vec{r}-\imath E_k\tau-\imath E_k t']} e^{-\eta\tau} \left\{ \int_\rho^\infty dr'' e^{\imath\frac{r''^2}{2\tau}} r'' + \frac{1}{\rho} \int_0^\rho dr'' e^{\imath\frac{r''^2}{2\tau}} r''^2 \right\} \quad (3.52)$$

integration by parts gives

$$\Phi_f^{(1)}(\vec{r}, t) = \imath \int_t^\infty dt' \frac{4\pi Z}{(2\pi\imath)^{\frac{3}{2}} \tau^{\frac{1}{2}} \rho} e^{[\imath\vec{k}\cdot\vec{r}-\imath E_k\tau-\imath E_k t']} e^{-\eta\tau} \int_0^\rho dr'' e^{\imath\frac{r''^2}{2\tau}} \quad (3.53)$$

Now, we set $\rho\zeta = r''$ to obtain

$$\Phi_f^{(1)}(\vec{r}, t) = \imath \int_t^\infty dt' \frac{4\pi Z}{(2\pi\imath)^{\frac{3}{2}} \tau^{\frac{1}{2}}} e^{[\imath\vec{k}\cdot\vec{r}-\imath E_k\tau-\imath E_k t']} e^{-\eta\tau} \int_0^1 d\zeta e^{\imath\frac{\rho(t')^2\zeta^2}{2\tau}} \quad (3.54)$$

The integral over ζ is an integral representation of the error function erf(x) [71] and therefore we get

$$\Phi_f^{(1)}(\vec{r}, t) = \imath \int_t^\infty dt' \frac{4\pi Z}{(2\pi\imath)\rho(t')} e^{[\imath\vec{k}\cdot\vec{r}-\imath E_k\tau-\imath E_k t']} e^{-\eta\tau} \text{erf}[\rho(t', \tau)/\sqrt{2\imath\tau}] \quad (3.55)$$

where

$$\vec{\rho}(t', \tau) = \vec{\alpha}(t') + \vec{r} - \vec{k}\tau$$

Changing integration variable from t' to τ we have

$$\Phi_f^{(1)}(\vec{r}, t) = \imath e^{[\imath\vec{k}\cdot\vec{r}-\imath E_k t]} \int_0^\infty d\tau \frac{4\pi Z}{(2\pi\imath)\rho(t, \tau)} e^{\eta\tau} \text{erf}[\rho(t, \tau)/\sqrt{2\imath\tau}] \quad (3.56)$$

where it is understood that $\eta \rightarrow 0^-$.

If we let $\rho(\tau)$ denote $\rho(t, \tau)$ when $\alpha = 0$ then the regular, relevant function, $\Phi_f^{(1)}$, is the difference

$$\Phi_f^{(1)} = \imath e^{[\imath\vec{k}\cdot\vec{r}-\imath E_k t]} \int_0^\infty d\tau 4\pi Z e^{\eta\tau} \left[\frac{\text{erf}[\rho(t, \tau)/\sqrt{2\imath\tau}]}{\rho(t, \tau)} - \frac{\text{erf}[\rho(\tau)/\sqrt{2\imath\tau}]}{\rho(\tau)} \right] \quad (3.57)$$

$\Phi_{\vec{r}}^{(1)}$ is the regular, singularity free, component of $\Phi_{\vec{r}}^{(1)}$ which is relevant to the high energy electrons of the ATI spectrum. It is the solution to the integral equation

$$|\Phi_{\vec{r}}^{(1)}(t)\rangle = \int_t^\infty dt' G_o^{(-)}(t, t') [V_A(\vec{r} + \vec{\alpha}(t')) - V_A(\vec{r})] |\chi_{\vec{k}}(t')\rangle \quad (3.58)$$

If we define $W(\vec{r}, \vec{\alpha}(t))$ to be

$$W(\vec{r}, \vec{\alpha}(t)) = V_A(\vec{r}, \vec{\alpha}(t)) - V_A(\vec{r}) \quad (3.59)$$

so that

$$|\Phi_{\vec{r}}^{(1)}(t)\rangle = \int_t^\infty dt' G_o^{(-)}(t, t') [W(\vec{r} + \vec{\alpha}(t'))] |\chi_{\vec{k}}(t')\rangle \quad (3.60)$$

then we arrive at a significant physical implication. For $r \gg \alpha$, $W(\vec{r}, \vec{\alpha}) \approx \frac{-\vec{\alpha} \cdot \vec{r}}{r^2}$, which is a short range potential. This implies that *the high energy electrons of the ATI spectrum are due to a short range potential rescattering*; i.e., due to $W(\vec{r}, \vec{\alpha})$. The long-range Coulomb potential accounts for the low energy direct electrons.

The irregular component, $\Phi_{\text{ir}}^{(1)}$, which contributes to the low energy direct electrons is given by (see Eq. (3.38))

$$|\Phi_{\text{ir}}^{(1)}(t)\rangle = \int_t^\infty dt' G_o^{(-)}(t, t') V_A(\vec{r}) |\chi_{\vec{k}}(t')\rangle \quad (3.61)$$

Now the Schrödinger equation for a free electron in a Coulomb center is

$$(i\frac{\partial}{\partial t} - H_o - \lambda V_A)\Psi_A^{(-)} = 0 \quad (3.62)$$

where λ is a perturbation parameter, then the Coulomb scattering states $\Psi_A^{(-)}$ are given by

$$|\Psi_A^{(-)}\rangle = |\chi_{\vec{k}}\rangle e^{-i\pi a/2} \Gamma(1+a) {}_1F_1(-a, 1, -i(kr + \vec{k} \cdot \vec{r})) \quad (3.63)$$

where $a = i\lambda Z/k$. We can write $\Psi_A^{(-)}$ as a power series solution in the form

$$\Psi_A^{(-)} = \sum_{n=0}^{\infty} \lambda^n \Psi_A^{(n)} \quad (3.64)$$

Substituting Eq. (3.64) into Eq. (3.62) we obtain, in Dirac bra-ket notation, for $\Psi_A^{(0)}$ and $\Psi_A^{(1)}$

$$(i\frac{\partial}{\partial t} - H_o) |\Psi_A^{(0)}\rangle = 0 \quad (3.65)$$

$$(i\frac{\partial}{\partial t} - H_o) |\Psi_A^{(1)}\rangle = V_A |\Psi_A^{(0)}\rangle \quad (3.66)$$

For $|\Psi_A^{(0)}\rangle$, the solution is a plane wave $|\chi_{\vec{k}}\rangle$. For $|\Psi_A^{(1)}\rangle$, the solution is

$$|\Psi_A^{(1)}\rangle = \int_t^\infty dt' G_o^{(-)}(t, t') V_A(\vec{r}') |\chi_{\vec{k}}(t')\rangle \quad (3.67)$$

Comparing Eqs. (3.61) and (3.67) we conclude that $|\Psi_A^{(1)}\rangle \equiv |\Phi_{\text{ir}}^{(1)}\rangle$ and the solution is irregular. However, from the power series solution given by Eq. (3.64) we have

$$\Psi_A^{(n)} = \frac{\partial^n \Psi_A^{(-)}}{\partial \lambda^n} |_{\lambda=0} \quad (3.68)$$

and therefore

$$|\Phi_{\text{ir}}^{(1)}\rangle = |\Psi_A^{(1)}\rangle = \frac{\partial |\Psi_A^{(-)}\rangle}{\partial \lambda} |_{\lambda=0} \quad (3.69)$$

$|\Phi_{\text{ir}}^{(1)}\rangle$ as given by Eq. (3.69) is regular nonsingular solution. If we let $|\Phi_{\text{d}}^{(1)}\rangle$ denote the regularized $|\Phi_{\text{ir}}^{(1)}\rangle$ as given by Eq. (3.69) so that

$$|\Phi_{\text{d}}^{(1)}\rangle = \frac{\partial |\Psi_A^{(-)}\rangle}{\partial \lambda} |_{\lambda=0} \quad (3.70)$$

then combining Eqs. (3.60) and (3.70) we finally obtain

$$|\Phi_{\text{f}}^{(1)}\rangle = |\Phi_{\text{r}}^{(1)}\rangle + |\Phi_{\text{d}}^{(1)}\rangle \quad (3.71)$$

$$= \int_t^\infty dt' G_o^{(-)}(t, t') [W(\vec{r}') + \vec{\alpha}(t')] |\chi_{\vec{k}}(t')\rangle + \frac{\partial |\Psi_A^{(-)}\rangle}{\partial \lambda} |_{\lambda=0} \quad (3.72)$$

$\Phi_{\text{f}}^{(1)}$ as given by Eqs. (3.71) and (3.72) is nonsingular. $\Phi_{\text{d}}^{(1)}$ is the component which contributes to the low energy direct electrons, as emphasized by the subscript d, and it is due to the long-range Coulomb potential. $\Phi_{\text{r}}^{(1)}$ is the component which is relevant to the high energy electrons and it is due to rescattering by the short range potential $W(\vec{r}, \vec{\alpha})$, as emphasized by the subscript r.

Using Eqs. (3.72), (3.71), (3.34) and (3.29) then $\Psi_{\text{f}}^{(-)}$ is given by

$$|\Psi_{\text{f}}^{(-)}(t)\rangle \approx e^{-i \int^t d\tau V_L(\tau)} \left[|\Phi_{\text{f}}^{(0)}\rangle + |\Phi_{\text{r}}^{(1)}\rangle + |\Phi_{\text{d}}^{(1)}\rangle \right] \quad (3.73)$$

$$\approx e^{-i \int^t d\tau V_L(\tau)} \left[|\chi_{\vec{k}}(t)\rangle + \int_t^\infty dt' G_o^{(-)}(t, t') [W(\vec{r}') + \vec{\alpha}(t')] |\chi_{\vec{k}}(t')\rangle + \frac{\partial |\Psi_A^{(-)}\rangle}{\partial \lambda} |_{\lambda=0} \right] \quad (3.74)$$

where the subscript f consistently indicates a final state. Now, Eq. (3.3) reads

$$(S - 1)_{\text{fi}} = S_{\text{fi}}^{(0)} + S_{\text{fi}}^{(1)} \quad (3.75)$$

with

$$\begin{aligned} S_{\text{fi}}^{(0)} &= -\imath \int_{-\infty}^{\infty} dt \langle e^{-\imath \int^t d\tau V_L(\tau)} \Phi_{\text{f}}^{(0)} | V_L | \phi_i \rangle \\ &= -\imath \int_{-\infty}^{\infty} dt \langle \Psi_{\vec{k}}^{(\text{v})} | V_L | \phi_i \rangle \end{aligned} \quad (3.76)$$

and

$$S_{\text{fi}}^{(1)} = -\imath \int_{-\infty}^{\infty} dt \langle e^{-\imath \int^t d\tau V_L(\tau)} \Phi_{\text{r}}^{(1)} | V_L | \phi_i \rangle - \imath \int_{-\infty}^{\infty} dt \langle e^{-\imath \int^t d\tau V_L(\tau)} \Phi_{\text{d}}^{(1)} | V_L | \phi_i \rangle \quad (3.77)$$

where $\Phi_{\text{r}}^{(1)}$ and $\Phi_{\text{d}}^{(1)}$ are given by Eqs. (3.60) and (3.70) respectively. $S_{\text{fi}}^{(0)}$ as given by Eq. (3.76) is the KFR term and therefore

$$S_{\text{fi}}^{(0)} = 2\pi\imath \langle \vec{k} | \phi_i \rangle \sum_{n=n_0}^{\infty} (E_k + E_B) \delta(E_k + E_B + U_p - nw) f_n \quad (3.78)$$

To evaluate the second term on the right hand side of Eq. (3.77) we will assume that $\Phi_{\text{d}}^{(1)}$ is an approximate eigenstate of the operator $e^{-\imath \int^t d\tau V_L(\tau)}$. Proceeding as we did in evaluating the KFR term we obtain

$$S_{\text{d}}^{(1)} = -\imath \int_{-\infty}^{\infty} dt \langle e^{-\imath \int^t d\tau V_L(\tau)} \Phi_{\text{d}}^{(1)} | V_L | \phi_i \rangle = 2\pi\imath \langle \Phi_{\text{d}}^{(1)} | \phi_i \rangle \sum_{n=n_0}^{\infty} (E_k + E_B) \delta(E_k + E_B + U_p - nw) f_n \quad (3.79)$$

where

$$\langle \Phi_{\text{d}}^{(1)} | \phi_i \rangle = \frac{\partial}{\partial \lambda} \left\{ \sqrt{\frac{Z^3}{\pi}} \frac{e^{-\imath \pi a/2} \Gamma(1-a)}{(2\pi)^{\frac{3}{2}}} \int d\vec{r} {}_1F_1[a, 1, \imath(kr + \vec{k} \cdot \vec{r})] e^{-i\vec{k} \cdot \vec{r}} e^{-Zr} \right\}_{\lambda=0} \quad (3.80)$$

The space integral is a Nordsieck type integral [72] (see Appendix A). It is evaluated to give

$$\langle \Phi_{\text{d}}^{(1)} | \phi_i \rangle = \frac{\imath}{k} \langle \vec{k} | \phi_i \rangle [-\imath \pi/2 + \gamma + \ln(\frac{Z + \imath k}{Z - \imath k}) + \imath \frac{k}{Z}] \quad (3.81)$$

where γ is Euler's constant.

Finally, evaluating the first term on the right hand side of Eq. (3.77) gives $S_{\text{r}}^{(1)}$ as given by Eq. (3.27). Thus we have

$$-\imath \int_{-\infty}^{\infty} dt \langle e^{-\imath \int^t d\tau V_L(\tau)} \Phi_{\text{r}}^{(1)} | V_L | \phi_i \rangle = S_{\text{r}}^{(1)} \quad (3.82)$$

where

$$\begin{aligned}
S_r^{(1)} &= 2\pi i \sum_{n=n_o}^{\infty} \delta(E_k + E_B + U_p - nw) \int d\vec{q} \langle \vec{q} | \phi_i(\vec{r}) \rangle \langle \vec{k} | V_A | \vec{q} \rangle \\
&\times \sum_{m=n_o}^{\infty'} \frac{U_p - mw}{E_q + E_B + U_p - mw - i\eta} f_m g_{n-m}
\end{aligned} \tag{3.83}$$

and the prime on the summation symbol, \sum' indicates the term $m = n$ is excluded from the sum.

It is to be emphasized again that $S_r^{(1)}$ is the term of the S matrix which is relevant to the high energy electrons and it is due to rescattering by the short range potential, $W(\vec{r}, \vec{\alpha})$. n is the number of absorbed photons for ionization from the initial state to the intermediate continuum state with canonical momentum \vec{q} to the final continuum states with canonical momentum \vec{k} and m is the number of absorbed photons for ionization from the initial state to intermediate continuum states with canonical momentum \vec{q} . Since the term $m = n$ is excluded from the sum, then the integrand has simple poles corresponding to resonances representing the essential continuum states channels responsible for continuum-continuum transitions. States are essential if they are populated during the entire process of ATI. Basis states of the Hamiltonian are restricted to only essential states. These are continuum states which differ from each other by the energy of one photon of the laser field. Therefore, based on the method of essential states [65], it is justifiable to perform the integration over the variable $q = |\vec{q}|$ by means so called *pole approximation* [65,66] according to

$$\lim_{\eta \rightarrow 0} \int_0^{\infty} \frac{f(q) dE_q}{E_q + E_B + U_p - mw - i\eta} \approx +i\pi f(q_m) \tag{3.84}$$

where the variable $q_m = \sqrt{2(mw - E_B - U_p)}$ denoting the discrete values of photoelectron canonical momentum corresponding to the intermediate essential continuum states. These continuum essential states give the main (dominant) contribution to $S_r^{(1)}$ and this justifies ignoring the principal value of the integral, for the singular part is supposed to be quite sufficient for retaining the predominant contribution in $S_r^{(1)}$. Therefore Eq. (3.83) now reads,

$$S_r^{(1)} = 2\pi i \sum_{n=n_o} \delta(E_k + E_B + U_p - nw) \int d\Omega \sum_{m=n_o} \langle \vec{q}_m | \phi_i \rangle \langle \vec{k} | V_A | \vec{q}_m \rangle$$

$$\times \imath\pi(U_p - mw) q_m [f_m g_{n-m}]_{q_m} \quad (3.85)$$

where $[f_m g_{n-m}]_{q_m}$ means that the expression inside the bracket is to be evaluated at q_m .

For the continuum-continuum transitions to occur, the direct electron ionization channels have to occur first. From the classical considerations presented in chapter 1 the direct ionization electron channels extend up to $2U_p$; i.e., to $m = 3n_o$. Quantum mechanics softens that limit. Indeed, channels for appreciable direct electron ionization rates extend up to $\approx 3U_p$; i.e., up to $4n_o$ beyond which rates severely drop. Therefore, we can terminate the sum over m in Eq. (3.85) at a cutoff value. We choose this value to be $\approx 6n_o$.

If we define $T^{(0)}$, $T_d^{(1)}$ and $T_r^{(1)}$ to be

$$T^{(0)} = -\langle \vec{k} | \phi_i \rangle (E_k + E_B) f_n \quad (3.86)$$

$$T_d^{(1)} = -\frac{\imath}{k} \langle \vec{k} | \phi_i \rangle (E_k + E_B) f_n [-\imath\pi/2 + \gamma + \ln(\frac{Z + \imath k}{Z - \imath k}) + \imath \frac{k}{z}] \quad (3.87)$$

$$T_r^{(1)} = -\imath\pi \int d\Omega \sum_{m=n_o}^{m_{\text{cut}}} \langle \vec{q}_m | \phi_i \rangle \langle \vec{k} | V_A | \vec{q}_m \rangle (U_p - mw) q_m [f_m g_{n-m}]_{q_m} \quad (3.88)$$

so that

$$T_{\text{fi}}(n) = T^{(0)} + T_d^{(1)} + T_r^{(1)} \quad (3.89)$$

then Eq. (3.75), reads

$$(S - 1)_{\text{fi}} = -2\pi\imath \sum_{n=n_o}^{\infty} \delta(E_k + E_B + U_p - nw) T_{\text{fi}}(n) \quad (3.90)$$

and therefore the differential ionization rates $\omega_{\text{fi}}(n, \theta)$ for the absorption of n photons with momentum \vec{k} making an angle θ with a fixed z axis in space, (Eq. (2.94)), is given by

$$\omega_{\text{fi}}(n, \theta) = 2\pi k(n) |T_{\text{fi}}(n, \theta)|^2 \quad (3.91)$$

In the following subsections we will give an explicit expressions for the Fourier components f_n , f_m , and g_{n-m} for both cases of circularly and linearly polarized light.

3.1.2 The Case of Circularly Polarized Electromagnetic Fields

The vector potential in the long wavelength approximation for a plane wave propagating along the z axis is

$$\vec{A}(t) = \frac{A_o}{\sqrt{2}} (\cos wt \hat{x} \pm \sin wt \hat{y}) \quad (3.92)$$

The Fourier components f_n have been calculated in chapter 2 and they are given in terms of Bessel functions. we have

$$f_n = (-1)^n e^{\pm i n \varphi_k} J_n\left(\frac{\sqrt{2U_p}}{w} k \sin \theta_k\right) \quad (3.93)$$

$$f_m = (-1)^m e^{\pm i m \varphi_q} J_m\left(\frac{\sqrt{2U_p}}{w} q \sin \theta_q\right) \quad (3.94)$$

$$g_{n-m} = (-1)^{n-m} e^{\pm i(n-m)\varphi_p} J_{n-m}\left(\frac{\sqrt{2U_p}}{w} p \sin \theta_p\right) \quad (3.95)$$

where $\vec{p} = \vec{k} - \vec{q}$ and $q = q_m = \sqrt{2(mw - E_B - U_p)}$

3.1.3 The Case of Linearly Polarized Electromagnetic Fields

The vector potential for a monochromatic linearly polarized plane wave in the long wavelength approximation is

$$\vec{A}(t) = A_o \hat{\epsilon} \cos wt \quad (3.96)$$

The Fourier components have been calculated in chapter 2. f_n is given in terms of generalized Bessel function whereas g_n is in terms of Bessel functions. We have

$$f_n = (-1)^n J_n\left(\frac{2\sqrt{U_p}}{w} k \cos \theta_k, -\frac{U_p}{2w}\right) \quad (3.97)$$

$$f_m = (-1)^m J_m\left(\frac{2\sqrt{U_p}}{w} q \cos \theta_q, -\frac{U_p}{2w}\right) \quad (3.98)$$

$$g_{n-m} = (-1)^{n-m} J_{n-m}\left(\frac{2\sqrt{U_p}}{w} [k \cos \theta_k - q \cos \theta_q]\right) \quad (3.99)$$

where $q = q_m = \sqrt{2(mw - E_B - U_p)}$ and the z axis is taken along the polarization vector $\hat{\epsilon}$.

3.2 An *ad hoc* Formulation of Above Threshold Ionization

We have concluded from an *ab initio* formulation of rescattering that high energy electrons of the ATI spectrum are due to short range potential rescattering and that the long-range Coulomb potential influence the low energy direct electrons of ATI spectrum. Based on this we will present a formulation of above threshold ionization in which we will

assume that the atomic potential V_A splits into two parts: a long-range Coulomb potential V_c and a short range potential V_s so that

$$V_A = V_c + V_s \quad (3.100)$$

and it is the rescattering by V_s which is relevant to the high energy electrons of ATI spectrum. Furthermore, the final continuum state of the electron, which is the solution of

$$(i\frac{\partial}{\partial t} - H_o - V_c - V_L)\Psi_{\vec{k}}^{(c)} = 0 \quad (3.101)$$

is assumed to be given by either by the Coulomb-Volkov wave function $\Psi_{\vec{k}}^{(cv)}$, introduced earlier by Jain and Tzoar [47]

$$\Psi_{\vec{k}}^{(cv)} = e^{-iS(\vec{k},t)} e^{\pi a/2} \Gamma(1 + ia) |\vec{k}\rangle_1 F_1(-ia, 1, -i(kr + \vec{k} \cdot \vec{r})) \quad (3.102)$$

where $a = Z/k$, or by an improved version of the Coulomb-Volkov wave function which is called the improved Coulomb-Volkov state ansatz [49-56,57-59]

$$\Psi_{\vec{Q}}^{(icv)} = e^{-iS(\vec{k},t)} e^{\pi a/2} \Gamma(1 + ia) |\vec{k}\rangle_1 F_1(-ia, 1, -i(Qr + \vec{Q} \cdot \vec{r})) \quad (3.103)$$

where $\vec{Q} = \vec{k} + \frac{1}{c}\vec{A}$ and $a = Z/Q$. Both of these wave functions include both V_L and the Coulomb potential to all orders. If we set $a = 0$ in $\Psi^{(c)}$ we get the Volkov state, $\Psi_{\vec{k}}^{(v)}$, which is to all orders in V_L but zero order in the Coulomb potential and we reproduce the KFR theory.

Now, the wave function $\Psi^{(-)}$ of the complete system which is the solution of Eq. (3.1) is expressed, in Dirac bra-ket notation, as

$$|\Psi_f^{(-)}(t)\rangle = |\Psi^{(c)}(t)\rangle + \int_t^\infty dt' G_c^{(-)}(t, t') V_s(t') |\Psi_f^{(-)}(t')\rangle \quad (3.104)$$

where the propagator $G_c^{(-)}(t, t')$ satisfies

$$(i\frac{\partial}{\partial t} - H_o - V_c - V_L)G_c^{(-)}(t, t') = \delta(t - t') \quad (3.105)$$

Within the strong field approximation (SFA), where $U_p \gg E_B$, we replace $\Psi^{(-)}$ on the right hand side of Eq. (3.104) by $\Psi^{(c)}$ and $G_c^{(-)}$ by $G_L^{(-)}$ and therefore we obtain

$$|\Psi_f^{(-)}(t)\rangle \approx |\Psi^{(c)}(t)\rangle + \int_t^\infty dt' G_L^{(-)}(t, t') V_s(t') |\Psi^{(c)}(t')\rangle \quad (3.106)$$

The scattering matrix $(S - 1)_{\text{fi}}$, as given by Eq. (3.3), now reads

$$(S - 1)_{\text{fi}} \approx -\imath \int_{-\infty}^{\infty} dt \langle \Psi^{(c)} | V_L \phi_i \rangle - \imath \int_{-\infty}^{\infty} dt \int_{-\infty}^t dt' \langle \Psi^{(c)} | V_s G_L^{(+)}(t, t') V_L(t') \phi_i(t') \rangle \quad (3.107)$$

setting $\tau = t - t'$ yields

$$(S - 1)_{\text{fi}} \approx -\imath \int_{-\infty}^{\infty} dt \langle \Psi^{(c)} | V_L \phi_i \rangle - \imath \int_{-\infty}^{\infty} dt \int_0^{\infty} d\tau \langle \Psi^{(c)} | V_s G_L^{(+)}(t, t - \tau) V_L(t - \tau) \phi_i(t - \tau) \rangle \quad (3.108)$$

Substituting for $G_L^{(+)}(t, t - \tau)$ using Eq. (3.10) we obtain

$$\begin{aligned} (S - 1)_{\text{fi}} &\approx -\imath \int_{-\infty}^{\infty} dt \langle \Psi^{(c)} | V_L \phi_i \rangle \\ &- \imath \int_{-\infty}^{\infty} dt \int_0^{\infty} d\tau \int d\vec{q} (-\imath) \langle \Psi^{(c)}(t) | V_s | \Psi_{\vec{q}}^{(v)}(t) \rangle \\ &\times \langle \Psi_{\vec{q}}^{(v)}(t - \tau) | V_L(t - \tau) \phi_i(t - \tau) \rangle e^{-\eta\tau} \end{aligned} \quad (3.109)$$

where $\eta \rightarrow 0^+$ is implied by the outgoing boundary conditions. The first term on the right hand side of Eq. (3.109) is the direct electron term and we denote it by $S_{\text{fi}}^{(0)}$

$$S_{\text{fi}}^{(0)} = -\imath \int_{-\infty}^{\infty} dt \langle \Psi^{(c)} | V_L \phi_i \rangle \quad (3.110)$$

It constitutes a generalized KFR theory, since unlike the KFR theory, the Coulomb effects are taken to all orders. The second term is the rescattering term which is relevant to the high energy electrons and its due to rescattering by the short range potential V_s and we denote by $S_{\text{fi}}^{(1)}$

$$S_{\text{fi}}^{(1)} = -\imath \int_{-\infty}^{\infty} dt \int_0^{\infty} d\tau \int d\vec{q} (-\imath) \langle \Psi^{(c)}(t) | V_s | \Psi_{\vec{q}}^{(v)}(t) \rangle \langle \Psi_{\vec{q}}^{(v)}(t - \tau) | V_L(t - \tau) \phi_i(t - \tau) \rangle e^{-\eta\tau} \quad (3.111)$$

In the following subsections we will evaluate in details both of the generalized direct term $S_{\text{fi}}^{(0)}$ (generalized KFR theory) and the generalized rescattering term $S_{\text{fi}}^{(1)}$.

3.2.1 Evaluation of the Generalized Direct Term

In the expression for $S_{\text{fi}}^{(0)}$ we will take $\Psi^{(c)}$ to be the improved Coulomb-Volkov wave-function $\Psi_{\vec{Q}}^{(\text{icv})}$. Substituting Eq. (3.103) for $\Psi_{\vec{Q}}^{(\text{icv})}$ into Eq. (3.110) we get

$$S_{\text{fi}}^{(0)} = -\iota \sqrt{\frac{Z^3}{\pi}} N_{\text{a}}^* \int_{-\infty}^{\infty} dt e^{\iota S(\vec{k}, t)} e^{\iota E_{\text{B}} t} \int d\vec{r} e^{-\iota \vec{k} \cdot \vec{r}} {}_1F_1[\iota a, 1, \iota(Qr + \vec{Q} \cdot \vec{r})] \left\{ \frac{1}{c} \vec{A} \cdot (-\iota \vec{\nabla}) + \frac{A^2}{2c^2} \right\} e^{-Zr} \quad (3.112)$$

where

$$\begin{aligned} \vec{Q} &= \vec{k} + \frac{1}{c} \vec{A} \\ N_{\text{a}} &= \frac{1}{(2\pi)^{\frac{3}{2}}} e^{\pi a/2} \Gamma(1 + \iota a) \\ a &= Z/Q \end{aligned} \quad (3.113)$$

For a linearly polarized light along the z axis, the vector potential is

$$\vec{A}(t) = A(t) \hat{z} = A_0 \hat{z} \cos \omega t \quad (3.114)$$

Then

$$\frac{1}{c} \vec{A} \cdot (-\iota \vec{\nabla}) = \frac{-\iota A(t)}{c} \frac{\partial}{\partial z} \quad (3.115)$$

$S_{\text{fi}}^{(0)}$ is given by

$$S_{\text{fi}}^{(0)} = -\iota \sqrt{\frac{Z^3}{\pi}} N_{\text{a}}^* \int_{-\infty}^{\infty} dt e^{\iota S(\vec{k}, t)} e^{\iota E_{\text{B}} t} \left(\frac{-ZA(t)}{c} I_1 + \frac{A^2}{2c^2} I_2 \right) \quad (3.116)$$

where

$$I_1 = \int d\vec{r} e^{[-\iota \vec{k} \cdot \vec{r} - Zr]} \frac{(-\iota z)}{r} {}_1F_1[\iota a, 1, \iota(Qr + \vec{Q} \cdot \vec{r})] = \frac{\partial}{\partial k_z} (J) \quad (3.117)$$

and

$$I_2 = \int d\vec{r} e^{[-\iota \vec{k} \cdot \vec{r} - Zr]} {}_1F_1[\iota a, 1, \iota(Qr + \vec{Q} \cdot \vec{r})] = -\frac{\partial}{\partial Z} (J) \quad (3.118)$$

In Eqs. (3.117) and (3.118) J is a Nordsieck type integral [72] (see Appendix A)

$$J = \int d\vec{r} e^{[-\iota \vec{k} \cdot \vec{r} - Zr]} \frac{1}{r} {}_1F_1[\iota a, 1, \iota(Qr + \vec{Q} \cdot \vec{r})] \quad (3.119)$$

which is evaluated to be

$$J = \frac{4\pi}{Z^2 + k^2} \left[\frac{(\vec{Q} - \vec{k})^2 - (Q + iZ)^2}{Z^2 + k^2} \right]^{-ia} \quad (3.120)$$

so that

$$I_1 = 8\pi \left[\frac{Z^2 + k^2}{(\vec{Q} - \vec{k})^2 + (Q + iZ)^2} \right]^{ia} \left\{ (ia - 1)k_z(Z^2 + k^2)^{-2} - ia(Q_z - k_z)(Z^2 + k^2)^{-1} [(\vec{Q} - \vec{k})^2 + (Q + iZ)^2]^{-1} \right\} \quad (3.121)$$

and

$$I_2 = -8\pi \left[\frac{Z^2 + k^2}{(\vec{Q} - \vec{k})^2 + (Q + iZ)^2} \right]^{ia} \left\{ (ia - 1)Z(Z^2 + k^2)^{-2} - ia(Q + iZ)(Z^2 + k^2)^{-1} [(\vec{Q} - \vec{k})^2 + (Q + iZ)^2]^{-1} \right\} \quad (3.122)$$

If we define ζ and ξ to be

$$\xi = Z^2 + k^2 \quad (3.123)$$

$$\zeta = (\vec{Q} - \vec{k})^2 + (Q + iZ)^2 \quad (3.124)$$

then from Eq. (3.116) for $S_{\text{fi}}^{(0)}$ we have

$$S_{\text{fi}}^{(0)} = 8\pi \sqrt{\frac{Z^3}{\pi}} N_{\text{a}}^* \int_{-\infty}^{\infty} dt e^{iS[k,t]} e^{iE_{\text{B}}t} \left(\frac{\xi}{\zeta} \right)^{ia} \times \left\{ \frac{ZA(t)}{c} [(ia - 1)k_z \xi^{-2} - ia(Q_z - k_z) \xi^{-1} \zeta^{-1}] + \frac{A^2}{2c^2} [(ia - 1)Z \xi^{-2} - ia(Q + iZ) \xi^{-1} \zeta^{-1}] \right\} \quad (3.125)$$

If we set $\vec{Q} = \vec{k}$ in Eq. (3.125), we obtain $S_{\text{fi}}^{(0)}$ had we used the Coulomb-Volkov wave function, and if we set $a = 0$ we reproduce the KFR theory.

Now, the integrand is periodic function of t and can be expanded in Fourier series so that the integral over t is easily performed to obtain

$$S_{\text{fi}}^{(0)} = -2\pi i \sum_{n=n_0}^{\infty} \delta(E_k + E_{\text{B}} + U_{\text{p}} - nw) T_{\text{fi}}^{(0)}(n) \quad (3.126)$$

where

$$\begin{aligned}
 T_{\text{fi}}^{(0)}(n) &= -8\pi\sqrt{\frac{Z^3}{\pi}}N_{\text{a}}^*\frac{1}{2\pi}\int_0^{2\pi}d\varphi e^{[i\frac{2\sqrt{U_{\text{p}}}}{w}k_z\sin\varphi+i\frac{U_{\text{p}}}{2w}\sin 2\varphi+n\varphi]}\left(\frac{\xi}{\zeta}\right)^{ia} \\
 &\times\left\{\frac{ZA(\varphi)}{c}[(ia-1)k_z\xi^{-2}-ia(Q_z-k_z)\xi^{-1}\zeta^{-1}] \right. \\
 &\left. +\frac{A^2(\varphi)}{2c^2}[(ia-1)Z\xi^{-2}-ia(Q+iZ)\xi^{-1}\zeta^{-1}]\right\}
 \end{aligned} \tag{3.127}$$

and $\varphi = wt$.

3.2.2 Evaluation of the Rescattering Term

We recall the Rescattering term $S_{\text{fi}}^{(1)}$

$$S_{\text{fi}}^{(1)} = -i\int_{-\infty}^{\infty}dt\int_0^{\infty}d\tau\int d\vec{q}(-i)\langle\Psi_{\vec{Q}}^{(\text{icv})}(t)|V_{\text{s}}|\Psi_{\vec{q}}^{(\text{v})}(t)\rangle\langle\Psi_{\vec{q}}^{(\text{v})}(t-\tau)|V_{\text{L}}(t-\tau)\phi_{\text{i}}(t-\tau)\rangle e^{-\eta\tau} \tag{3.128}$$

where we used $\Psi_{\vec{Q}}^{(\text{icv})}$ for $\Psi^{(\text{c})}$. The Volkov state $|\Psi_{\vec{q}}^{(\text{v})}\rangle$ is expressed as

$$|\Psi_{\vec{q}}^{(\text{v})}\rangle = e^{-iS(\vec{q},t)}|\vec{q}\rangle \tag{3.129}$$

Therefore substituting into Eq. (3.128) we obtain

$$S_{\text{fi}}^{(1)} = -i\int_{-\infty}^{\infty}dt\int_0^{\infty}d\tau\int d\vec{q}(-i)\langle\Psi_{\vec{Q}}^{(\text{icv})}(t)|V_{\text{s}}|\vec{q}\rangle\langle\vec{q}|V_{\text{L}}(t-\tau)\phi_{\text{i}}(t-\tau)\rangle e^{-iS(\vec{q},t,\tau)} e^{-\eta\tau} \tag{3.130}$$

where

$$S(\vec{q},t,\tau) = \frac{1}{2}\int_{t-\tau}^t dt' [q + \frac{\vec{A}(t')}{c}]^2 \tag{3.131}$$

is the semiclassical action for the propagation of an electron from the moment of birth at $t - \tau$ to the moment of rescattering at t . Now, the integral over \vec{q} is evaluated analytically using the saddle-point method [Appendix B] to obtain

$$S_{\text{fi}}^{(1)} = -i\int_{-\infty}^{\infty}dt\int_0^{\infty}d\tau(-i)\langle\Psi_{\vec{Q}}^{(\text{icv})}(t)|V_{\text{s}}|\vec{q}_{\text{s}}\rangle\langle\vec{q}_{\text{s}}|V_{\text{L}}(t-\tau)\phi_{\text{i}}(t-\tau)\rangle e^{-iS(\vec{q}_{\text{s}},t,\tau)}\left(\frac{2\pi}{i\tau+\epsilon}\right)^{\frac{3}{2}}e^{-\eta\tau} \tag{3.132}$$

where

$$\vec{q}_{\text{s}} = \frac{1}{\tau}[\vec{\alpha}(t-\tau) - \vec{\alpha}(t)] \tag{3.133}$$

is the solution of $\vec{\nabla}_{\vec{q}} S(\vec{q}, t, \tau) = 0$, $\vec{\alpha}$ is given by Eq. (3.19) and the parameter ϵ is introduced to smooth the singularity in τ .

If we define $U(t)$ to be

$$U(t) = \frac{1}{2c^2} \int^t dt' A^2(t') = U_p t + U_1(t) \quad (3.134)$$

so that

$$S(\vec{q}, t, \tau) = \frac{1}{2} q^2 \tau + \vec{q} \cdot [\vec{\alpha}(t) - \vec{\alpha}(t - \tau)] + U(t) - U(t - \tau) \quad (3.135)$$

then

$$S(\vec{q}_s, t, \tau) = -\frac{1}{2} q_s^2 \tau + U(t) - U(t - \tau) \quad (3.136)$$

Writing

$$\begin{aligned} \phi_i(\vec{r}, t) &= e^{iE_B t} \phi_i(\vec{r}) \\ \Psi_{\vec{Q}}^{(\text{icv})}(\vec{r}, t) &= e^{-iS(\vec{k}, t)} \Psi_{\vec{Q}}^{(\text{icv})}(\vec{r}) \\ e^{-iS(\vec{k}, t)} &= e^{-i[E_k + \vec{k} \cdot \vec{\alpha} + U(t)]} \end{aligned}$$

therefore Eq. (3.132) now becomes

$$\begin{aligned} S_{\text{fi}}^{(1)} &= -i \int_{-\infty}^{\infty} dt e^{i[E_k + E_B + U_p]t} (-i) e^{i\vec{k} \cdot \vec{\alpha}(t)} \int_0^{\infty} d\tau \left(\frac{2\pi}{i\tau + \epsilon} \right)^{\frac{3}{2}} e^{i[\frac{1}{2}q_s^2 + U_1(t-\tau) - (E_B + U_p)\tau]} \\ &\quad \times \langle \Psi_{\vec{Q}}^{(\text{ivc})} | V_s | \vec{q}_s \rangle \langle \vec{q}_s | V_L(\vec{q}_s, t - \tau) | \phi_i \rangle e^{-\eta\tau} \end{aligned} \quad (3.137)$$

The integrand over t is periodic function of t with period $2\pi/w$ and therefore it can be expanded in a Fourier series so that

$$S_{\text{fi}}^{(1)} = -2\pi i \sum_{n=n_0}^{\infty} \delta(E_k + E_B + U_p - nw) T_{\text{fi}}^{(1)}(n) \quad (3.138)$$

where

$$\begin{aligned} T_{\text{fi}}^{(1)}(n) &= -\frac{i}{2\pi} \int_0^{2\pi} d\varphi e^{i[\vec{k} \cdot \vec{\alpha}(\varphi) + n\varphi]} \int_0^{\infty} d\tau \left(\frac{2\pi}{i\tau + \epsilon} \right)^{\frac{3}{2}} e^{i[\frac{1}{2}q_s^2 + U_1(\varphi-\tau) - (E_B + U_p)\tau]} \\ &\quad \times \langle \Psi_{\vec{Q}}^{(\text{ivc})} | V_s | \vec{q}_s \rangle \langle \vec{q}_s | \phi_i \rangle V_L(\vec{q}_s, \varphi - \tau) e^{-\eta\tau} \end{aligned} \quad (3.139)$$

and $\varphi = wt$. Now, the inner product $\langle \vec{q}_s | \phi_i \rangle$ is the Fourier transform of the initial ground state, ϕ_i

$$\phi_i(\vec{r}) = \sqrt{\frac{Z^3}{\pi}} e^{-Zr} \quad (3.140)$$

so that

$$\langle \vec{q}_s | \phi_i \rangle = \frac{1}{(2\pi)^{\frac{3}{2}}} \sqrt{\frac{Z^3}{\pi}} \int d\vec{r} e^{-i\vec{q}_s \cdot \vec{r} - Zr} = \frac{\sqrt{8Z^5}}{\pi} \frac{1}{(Z^2 + q_s^2)^2} \quad (3.141)$$

If the short range potential, V_s , is taken to be Yukawa type

$$V_s = -Z \frac{e^{-\lambda r}}{r} \quad (3.142)$$

then

$$\langle \Psi_{\vec{Q}}^{(\text{ivc})} | V_s | \vec{q}_s \rangle = \frac{-Z}{(2\pi)^{\frac{3}{2}}} N_a^* \int d\vec{r} e^{-i(\vec{k} - \vec{q}_s) \cdot \vec{r} - \lambda r} \frac{1}{r} {}_1F_1[\iota a, 1, \iota(Qr + \vec{Q} \cdot \vec{r})] \quad (3.143)$$

the above integral is similar to J evaluated in Eq. (3.119) and so we have

$$\langle \Psi_{\vec{Q}}^{(\text{ivc})} | V_s | \vec{q}_s \rangle = \frac{-Z}{(2\pi)^{\frac{3}{2}}} N_a^* \frac{4\pi}{\lambda^2 + (\vec{k} - \vec{q}_s)^2} \left[\frac{(\vec{Q} - [\vec{k} - \vec{q}_s])^2 - (Q + \iota\lambda)^2}{\lambda^2 + (\vec{k} - \vec{q}_s)^2} \right]^{-\iota a} \quad (3.144)$$

and since

$$V_L(\vec{q}_s, \varphi - \tau) = \frac{1}{c} \vec{A}(\varphi - \tau) \cdot \vec{q}_s + \frac{A^2(\varphi - \tau)}{2c^2} \quad (3.145)$$

Therefore Eq. (3.139) for $T_{\text{fi}}^{(1)}$ is written as

$$\begin{aligned} T_{\text{fi}}^{(1)}(n) &= -\frac{\iota}{2\pi} \left(\frac{-4Z^{\frac{7}{2}} N_a^*}{(\pi)^{\frac{3}{2}}} \right) \int_0^{2\pi} d\varphi e^{i[\vec{k} \cdot \vec{\alpha}(\varphi) + n\varphi]} \int_0^\infty d\tau \left(\frac{2\pi}{\iota\tau + \epsilon} \right)^{\frac{3}{2}} e^{i[\frac{1}{2}q_s^2 + U_1(\varphi - \tau) - (E_B + U_p)\tau]} \\ &\times \frac{1}{(Z^2 + q_s^2)^2} \frac{1}{\lambda^2 + (\vec{k} - \vec{q}_s)^2} \left[\frac{(\vec{Q} - [\vec{k} - \vec{q}_s])^2 - (Q + \iota\lambda)^2}{\lambda^2 + (\vec{k} - \vec{q}_s)^2} \right]^{-\iota a} \\ &\times \left[\frac{1}{c} \vec{A}(\varphi - \tau) \cdot \vec{q}_s + \frac{A^2(\varphi - \tau)}{2c^2} \right] e^{-\eta\tau} \end{aligned} \quad (3.146)$$

If we write

$$(S - 1)_{\text{fi}} \approx S_{\text{fi}}^{(0)} + S_{\text{fi}}^{(1)} = -2\pi\iota \sum_{n=n_0}^{\infty} \delta(E_k + E_B + U_p - nw) T_{\text{fi}}(n) \quad (3.147)$$

then the differential ionization rate, $w_{\text{fi}}(n, \theta)$, is

$$w_{\text{fi}} = 2\pi k_f(n) |T_{\text{fi}}(n)|^2 \quad (3.148)$$

where $k_f(n) = \sqrt{2(nw - U_p - E_B)}$ and

$$T_{\text{fi}}(n) = T_{\text{fi}}^{(0)}(n) + T_{\text{fi}}^{(1)}(n)$$

$$\begin{aligned}
T_{\text{fi}}^{(0)}(n) &= -8\pi\sqrt{\frac{Z^3}{\pi}}N_{\text{a}}^*\frac{1}{2\pi}\int_0^{2\pi}d\varphi e^{[i\frac{2\sqrt{U_{\text{p}}}}{w}k_z\sin\varphi+i\frac{U_{\text{p}}}{2w}\sin 2\varphi+n\varphi]}\left(\frac{\xi}{\zeta}\right)^{ia} \\
&\quad \times \left\{ \frac{ZA(\varphi)}{c}[(ia-1)k_z\xi^{-2}-ia(Q_z-k_z)\xi^{-1}\zeta^{-1}] + \right. \\
&\quad \left. \frac{A^2(\varphi)}{2c^2}[(ia-1)Z\xi^{-2}-ia(Q+iZ)\xi^{-1}\zeta^{-1}] \right\} \\
T_{\text{fi}}^{(1)}(n) &= -\frac{i}{2\pi}\left(\frac{-4Z^{\frac{7}{2}}N_{\text{a}}^*}{(\pi)^{\frac{3}{2}}}\right)\int_0^{2\pi}d\varphi e^{i[\vec{k}\cdot\vec{\alpha}(\varphi)+n\varphi]}\int_0^\infty d\tau\left(\frac{2\pi}{i\tau+\epsilon}\right)^{\frac{3}{2}}e^{i[\frac{1}{2}q_{\text{s}}^2+U_1(\varphi-\tau)-(E_{\text{B}}+U_{\text{p}})\tau]} \\
&\quad \times \frac{1}{(Z^2+q_{\text{s}}^2)^2}\frac{1}{\lambda^2+(\vec{k}-\vec{q}_{\text{s}})^2}\left[\frac{(\vec{Q}-[\vec{k}-\vec{q}_{\text{s}}])^2-(Q+i\lambda)^2}{\lambda^2+(\vec{k}-\vec{q}_{\text{s}})^2}\right]^{-ia} \\
&\quad \times \left[\frac{1}{c}\vec{A}(\varphi-\tau)\cdot\vec{q}_{\text{s}}+\frac{A^2(\varphi-\tau)}{2c^2}\right]e^{-\eta\tau}
\end{aligned} \tag{3.149}$$

ξ , ζ and \vec{q}_{s} are given by Eqs. (3.123), (3.124), and (3.133) respectively and $\vec{Q} = \vec{k} + \frac{\vec{A}}{c}$.

Eqs. (3.148) and (3.149) represent a generalized S matrix formulation of above threshold ionization including rescattering with Coulomb effects taken to all orders. If we set $a = 0$, then the formulation reduces to rescattering only with no Coulomb effects, which should be adequate to account for the high energy plateau of ATI.

3.2.3 Rescattering Considerations with No Coulomb Effects

Rather than setting $a = 0$ in Eqs. (3.148) and (3.149), we will follow an equivalent approach, which enable us to further simplify these equation into more compact form. Rescattering considerations only with no Coulomb effects means that the solution $\Psi_{\text{f}}^{(-)}$ of Eq. (3.1) is approximately written as

$$|\Psi_{\text{f}}^{(-)}(t)\rangle \approx |\Psi_{\text{k}}^{(\text{v})}(t)\rangle + \int_t^\infty dt' G_{\text{L}}^{(-)}(t, t')V_{\text{A}}|\Psi_{\text{k}}^{(\text{v})}(t')\rangle \tag{3.150}$$

so that

$$(S-1)_{\text{fi}} \approx S_{\text{fi}}^{(0)} + S_{\text{fi}}^{(1)} \tag{3.151}$$

where

$$S_{\text{fi}}^{(0)} = -i\int_{-\infty}^\infty dt \langle \Psi_{\text{k}}^{(\text{v})} | V_{\text{L}}\phi_{\text{i}} \rangle \tag{3.152}$$

$$S_{\text{fi}}^{(1)} = -\imath \int_{-\infty}^{\infty} dt \int_{-\infty}^t dt' \langle \Psi_{\vec{k}}^{(v)} | V_A G_L^{(+)}(t, t') V_L(t') | \phi_i(t') \rangle \quad (3.153)$$

Now, If we write

$$V_L = (H_o + V_L) - (H_o + V_A) + V_A \quad (3.154)$$

and, since

$$\begin{aligned} (H_o + V_L) | \Psi_{\vec{k}}^{(v)} \rangle &= \imath \frac{\partial}{\partial t} | \Psi_{\vec{k}}^{(v)} \rangle \\ (H_o + V_A) | \phi_i \rangle &= -E_B | \phi_i \rangle \end{aligned}$$

then via integration by parts $S_{\text{fi}}^{(0)}$ and $S_{\text{fi}}^{(1)}$ can be written as

$$S_{\text{fi}}^{(0)} = -\imath \int_{-\infty}^{\infty} dt \langle \Psi_{\vec{k}}^{(v)} | V_A \phi_i \rangle \quad (3.155)$$

$$S_{\text{fi}}^{(1)} = -S_{\text{fi}}^{(0)} - \imath \int_{-\infty}^{\infty} dt \int_{-\infty}^t dt' \langle \Psi_{\vec{k}}^{(v)} | V_A G_L^{(+)}(t, t') V_A(t') | \phi_i(t') \rangle \quad (3.156)$$

and therefore

$$(S - 1)_{\text{fi}} \approx S_{\text{fi}}^{(0)} + S_{\text{fi}}^{(1)} = -\imath \int_{-\infty}^{\infty} dt \int_{-\infty}^t dt' \langle \Psi_{\vec{k}}^{(v)} | V_A G_L^{(+)}(t, t') V_A(t') | \phi_i(t') \rangle \quad (3.157)$$

Since the high energy electrons plateau of the ATI spectrum is due to short range potential rescattering, we will replace V_A with the short range Yukawa type potential V_s .

Thus we obtain

$$(S - 1)_{\text{fi}} \approx -\imath \int_{-\infty}^{\infty} dt \int_{-\infty}^t dt' \langle \Psi_{\vec{k}}^{(v)} | V_s G_L^{(+)}(t, t') V_s(t') | \phi_i(t') \rangle \quad (3.158)$$

where

$$V_s = -Z \frac{e^{-\lambda r}}{r} \quad (3.159)$$

We will proceed similarly to what we did earlier. Thus substituting for $G_L^{(+)}(t, t')$ using Eq. (3.10) and setting $\tau = t - t'$ we obtain

$$(S - 1)_{\text{fi}} \approx -\imath \int_{-\infty}^{\infty} dt \int_0^{\infty} d\tau \int d\vec{q} (-\imath) \langle \Psi_{\vec{k}}^{(v)}(t) | V_s | \Psi_{\vec{q}}^{(v)}(t) \rangle \langle \Psi_{\vec{q}}^{(v)}(t - \tau) | V_s | \phi_i(t - \tau) \rangle e^{-\eta\tau} \quad (3.160)$$

Now, the Volkov state, $|\Psi_{\vec{q}}^{(v)}\rangle$, is expressed as

$$|\Psi_{\vec{q}}^{(v)}\rangle = e^{-\imath S(\vec{q}, t)} | \vec{q} \rangle \quad (3.161)$$

Therefore substituting int Eq. (3.160) we obtain

$$(S-1)_{\text{fi}} \approx -\iota \int_{-\infty}^{\infty} dt \int_0^{\infty} d\tau \int d\vec{q} (-\iota) \langle \Psi_{\vec{k}}^{(\text{v})}(t) | V_{\text{s}} | \vec{q} \rangle \langle \vec{q} | V_{\text{s}} \phi_{\text{i}}(t-\tau) \rangle e^{-\iota S(\vec{q}, t, \tau)} e^{-\eta\tau} \quad (3.162)$$

where

$$S(\vec{q}, t, \tau) = \frac{1}{2} \int_{t-\tau}^t dt' [q + \frac{\vec{A}(t')}{c}]^2 \quad (3.163)$$

is the semiclassical action for the propagation of an electron from the moment of birth at $t - \tau$ to the moment of rescattering at t . Now, the integral over \vec{q} is evaluated analytically using the saddle-point method [Appendix B] to obtain

$$(S-1)_{\text{fi}} \approx -\iota \int_{-\infty}^{\infty} dt \int_0^{\infty} d\tau (-\iota) \langle \Psi_{\vec{k}}^{(\text{v})}(t) | V_{\text{s}} | \vec{q}_{\text{s}} \rangle \langle \vec{q}_{\text{s}} | V_{\text{s}} \phi_{\text{i}}(t-\tau) \rangle e^{-\iota S(\vec{q}_{\text{s}}, t, \tau)} \left(\frac{2\pi}{\iota\tau + \epsilon} \right)^{\frac{3}{2}} e^{-\eta\tau} \quad (3.164)$$

where

$$\vec{q}_{\text{s}} = \frac{1}{\tau} [\vec{\alpha}(t - \tau) - \vec{\alpha}(t)] \quad (3.165)$$

is the solution of $\vec{\nabla}_{\vec{q}} S(\vec{q}, t, \tau) = 0$, $\vec{\alpha}$ is given by Eq. (3.19) and the parameter ϵ is introduced to smooth the singularity in τ .

If we define $U(t)$ to be

$$U(t) = \frac{1}{2c^2} \int^t dt' A^2(t') = U_{\text{p}}t + U_1(t) \quad (3.166)$$

so that

$$S(\vec{q}, t, \tau) = \frac{1}{2} q^2 \tau + \vec{q} \cdot [\vec{\alpha}(t) - \vec{\alpha}(t - \tau)] + U(t) - U(t - \tau) \quad (3.167)$$

then

$$S(\vec{q}_{\text{s}}, t, \tau) = -\frac{1}{2} q_{\text{s}}^2 \tau + U(t) - U(t - \tau) \quad (3.168)$$

Writing

$$\begin{aligned} \phi_{\text{i}}(\vec{r}, t) &= e^{\iota E_{\text{B}}t} \phi_{\text{i}}(\vec{r}) \\ | \Psi_{\vec{k}}^{(\text{v})} \rangle &= e^{-\iota S(\vec{k}, t)} | \vec{q} \rangle \\ e^{-\iota S(\vec{k}, t)} &= e^{-\iota [E_{\text{k}} + \vec{k} \cdot \vec{\alpha} + U(t)]} \end{aligned}$$

therefore Eq. (3.164) now becomes

$$(S-1)_{\text{fi}} \approx -\imath \int_{-\infty}^{\infty} dt e^{\imath[E_k + E_B + U_P]t} (-\imath) e^{\imath \vec{k} \cdot \vec{\alpha}(t)} \int_0^{\infty} d\tau \left(\frac{2\pi}{\imath\tau + \epsilon} \right)^{\frac{3}{2}} e^{\imath[\frac{1}{2}q_s^2 + U_1(t-\tau) - (E_B + U_P)\tau]} \times \langle \vec{k} | V_s | \vec{q}_s \rangle \langle \vec{q}_s | V_s | \phi_i \rangle e^{-\eta\tau} \quad (3.169)$$

The integrand for the integration over t is periodic function of t with period $2\pi/w$ and therefore it can be expanded in a Fourier series so that

$$(S-1)_{\text{fi}} \approx -2\pi\imath \sum_{n=n_0}^{\infty} \delta(E_k + E_B + U_P - nw) T_{\text{fi}}(n) \quad (3.170)$$

where

$$T_{\text{fi}}(n) = -\frac{\imath}{2\pi} \int_0^{2\pi} d\varphi e^{\imath[\vec{k} \cdot \vec{\alpha}(\varphi) + n\varphi]} \int_0^{\infty} d\tau \left(\frac{2\pi}{\imath\tau + \epsilon} \right)^{\frac{3}{2}} e^{\imath[\frac{1}{2}q_s^2 + U_1(\varphi-\tau) - (E_B + U_P)\tau]} \times \langle \vec{k} | V_s | \vec{q}_s \rangle \langle \vec{q}_s | V_s | \phi_i \rangle e^{-\eta\tau} \quad (3.171)$$

and $\varphi = wt$.

Now, the initial ground state $\phi_i(\vec{r})$ is

$$\phi_i(\vec{r}) = \sqrt{\frac{Z^3}{\pi}} e^{-Zr} \quad (3.172)$$

the short range Yukawa type potential, V_s , is

$$V_s = -Z \frac{e^{-\lambda r}}{r} \quad (3.173)$$

thus we have

$$\langle \vec{q}_s | V_s | \phi_i \rangle = -\frac{1}{(2\pi)^{\frac{3}{2}}} \sqrt{\frac{Z^3}{\pi}} \int d\vec{r} e^{-\imath \vec{q}_s \cdot \vec{r} - Zr} \frac{e^{-\lambda r}}{r} = -\frac{\sqrt{2Z^5}}{\pi} \frac{1}{\vec{q}_s^2 + (Z + \lambda)^2} \quad (3.174)$$

and

$$\langle \vec{k} | V_s | \vec{q}_s \rangle = -\frac{Z}{(2\pi)^3} \int d\vec{r} e^{-\imath(\vec{k} - \vec{q}_s) \cdot \vec{r}} \frac{e^{-\lambda r}}{r} = -\frac{Z}{2\pi^2} \frac{1}{(\vec{k} - \vec{q}_s)^2 + \lambda^2} \quad (3.175)$$

Therefore, Eq. (3.171), for $T_{\text{fi}}(n)$ reads

$$T_{\text{fi}}(n) = -\frac{\imath}{2\pi} \int_0^{2\pi} d\varphi e^{\imath[\vec{k} \cdot \vec{\alpha}(\varphi) + n\varphi]} \int_0^{\infty} d\tau \left(\frac{2\pi}{\imath\tau + \epsilon} \right)^{\frac{3}{2}} e^{\imath[\frac{1}{2}q_s^2 + U_1(\varphi-\tau) - (E_B + U_P)\tau]} \times \frac{\sqrt{2Z^7}}{2\pi^3} \left[\frac{1}{\vec{q}_s^2 + (Z + \lambda)^2} \right] \left[\frac{1}{(\vec{k} - \vec{q}_s)^2 + \lambda^2} \right] e^{-\eta\tau} \quad (3.176)$$

For a linearly polarized electromagnetic field with polarization vector $\hat{\epsilon}$, the vector potential $\vec{A}(t)$ is

$$\vec{A}(t) = A_0 \hat{\epsilon} \cos wt \quad (3.177)$$

so we have

$$\vec{\alpha}(t) = \frac{A_0}{wc} \hat{\epsilon} \sin wt \quad (3.178)$$

$$U_1(t) = \frac{U_p}{2w} \sin 2wt \quad (3.179)$$

$$\vec{q}_s(\varphi, \tau) = \frac{2}{\tau w} \sqrt{U_p} \{ \sin(\varphi - w\tau) - \sin \varphi \} \hat{\epsilon} \quad (3.180)$$

$$\vec{k} \cdot \vec{\alpha} = \frac{2}{w} \sqrt{U_p} k \cos \theta \sin \varphi \quad (3.181)$$

where θ is the angle that the momentum \vec{k} of the ejected electron makes with the polarization vector $\hat{\epsilon}$. It is to be noticed that

$$\lim_{\tau \rightarrow 0} q_s = -2\sqrt{U_p} \cos \varphi \quad (3.182)$$

Substituting Eqs. (3.179–3.181) into Eq. (3.176) we finally obtain

$$\begin{aligned} T_{\text{fi}}(n) = & -\frac{i}{2\pi} \int_0^{2\pi} d\varphi e^{i[\frac{2}{w}\sqrt{U_p} k \cos \theta \sin \varphi + n\varphi]} \int_0^\infty d\tau \left(\frac{2\pi}{i\tau + \epsilon} \right)^{\frac{3}{2}} e^{i[\frac{1}{2}q_s^2 + \frac{U_p}{2w} \sin[2(\varphi - w\tau)] - (E_B + U_p)\tau]} \\ & \times \frac{\sqrt{2Z^7}}{2\pi^3} \left[\frac{1}{q_s^2 + (Z + \lambda)^2} \right] \left[\frac{1}{q_s^2 + k^2 - 2kq_s \cos \theta + \lambda^2} \right] e^{-\eta\tau} \end{aligned} \quad (3.183)$$

and therefore the differential ionization rate, $\omega_{\text{fi}}(n, \theta)$, for the absorption of n photons and making an angle θ with the polarization vector $\hat{\epsilon}$ is

$$\omega_{\text{fi}}(n, \theta) = 2\pi k(n) |T(n)_{\text{fi}}|^2 \quad (3.184)$$

with the energy conserving condition

$$k(n) = \sqrt{2E_k} = \sqrt{2(nw - U_p - E_B)} \quad (3.185)$$

Accurate numerical evaluations of Eq (3.149) or Eq. (3.183) is very cumbersome. The integrand is highly oscillatory in both φ and τ . In addition to being highly oscillatory, the integrand in τ is slowly decaying and the rapid oscillations extend to infinity. We will utilize a recently introduced method to evaluate the numerical integration over τ [67,68], and the integration over φ is carried out using the fast Fourier transform method [59].

3.3 An *ab initio* Generalized S Matrix Formulation of Above Threshold Ionization

In section (3.1) of this chapter we presented an *ab initio* formulation of above threshold ionization. In that *ab initio* formulation the long-range Coulomb potential is included only to first order. Based on it, we demonstrated that the long-range Coulomb potential affects the low energy photoelectrons. In this section we will generalize the *ab initio* formulation presented in section (3.1) to include the long-range Coulomb potential to all orders. The motivation behind this is that the recent experimental findings [73-75,78-79] and numerical solutions of the time dependent Schrödinger equation [76-77,80-81] confirm the importance of the long-range Coulomb potential on the low energy photoelectrons.

Our starting point will be Eq. (3.32), which is the equation of the complete system in the oscillating frame

$$\left[\imath \frac{\partial}{\partial t} - H_o - V_A(\vec{r} + \vec{\alpha}) \right] \Phi_f^{(-)} = 0 \quad (3.186)$$

Earlier we defined the time dependent short range potential $W(\vec{\alpha})$ to be

$$W(\vec{\alpha}) = V_A(\vec{r} + \vec{\alpha}) - V_A(\vec{r}) \quad (3.187)$$

so that Eq. (3.186) of the complete system in the oscillating frame is rewritten as

$$\left[\imath \frac{\partial}{\partial t} - H_o - V_A(\vec{r}) - W(\vec{\alpha}) \right] \Phi_f^{(-)} = 0 \quad (3.188)$$

and therefore the wave function $\Phi_f^{(-)}$ is expressed as

$$\Phi_f^{(-)}(t) = \Psi_{A,\vec{k}}^{(-)}(t) + \int_t^\infty dt' G_A^{(-)}(t, t') W(\vec{\alpha}(t')) \Phi_f^{(-)}(t') \quad (3.189)$$

where $\Psi_{A,\vec{k}}^{(-)}(t)$ is the solution of

$$\left(\imath \frac{\partial}{\partial t} - H_o - V_A \right) \Psi_{A,\vec{k}}^{(-)}(t) = 0 \quad (3.190)$$

which is given by

$$\Psi_{A,\vec{k}}^{(-)}(\vec{r}, t) = \frac{e^{\pi a/2} \Gamma(1 + ia)}{(2\pi)^{\frac{3}{2}}} {}_1F_1[-ia, 1, -\imath(kr + \vec{k} \cdot \vec{r})] e^{i\vec{k} \cdot \vec{r} - \imath E_k t} \quad (3.191)$$

and the advanced Coulomb Green function, $G_A^{(-)}(t, t')$, satisfies

$$\left(\imath \frac{\partial}{\partial t} - H_o - V_A\right) G_A^{(-)}(t, t') = \delta(t - t') \quad (3.192)$$

The solution of the complete system in the laboratory frame, $\Psi_f^{(-)}$, is obtained from $\Phi_f^{(-)}$ through

$$\Psi_f^{(-)} = e^{-\imath \int^t d\tau V_L(\tau)} \Phi_f^{(-)} \quad (3.193)$$

$$= e^{-\imath \int^t d\tau V_L(\tau)} \left\{ \Psi_{A, \vec{k}}^{(-)}(t) + \int_t^\infty dt' G_A^{(-)}(t, t') W(\vec{\alpha}(t')) \Phi_f^{(-)}(t') \right\} \quad (3.194)$$

within the strong field approximation (SFA), we replace $\Phi_f^{(-)}$ by $\Psi_{A, \vec{k}}^{(-)}$ so that

$$\begin{aligned} \Psi_f^{(-)} &= e^{-\imath \int^t d\tau V_L(\tau)} \Phi_f^{(-)} \\ &\approx e^{-\imath \int^t d\tau V_L(\tau)} \left\{ \Psi_{A, \vec{k}}^{(-)}(t) + \int_t^\infty dt' G_A^{(-)}(t, t') W(\vec{\alpha}(t')) \Psi_{A, \vec{k}}^{(-)}(t') \right\} \end{aligned} \quad (3.195)$$

Therefore Eq. (3.3) now reads

$$\begin{aligned} (S - 1)_{\text{fi}} &\approx -\imath \int_{-\infty}^\infty dt \langle e^{-\imath \int^t d\tau V_L(\tau)} \Psi_{A, \vec{k}}^{(-)} | V_L \phi_i \rangle \\ &\quad - \imath \int_{-\infty}^\infty dt \int_{-\infty}^t dt' \langle \Psi_{A, \vec{k}}^{(-)} | W(\vec{\alpha}) G_A^{(+)}(t, t') e^{\imath \int^{t'} d\tau V_L(\tau)} V_L | \phi_i \rangle \end{aligned} \quad (3.196)$$

Eq. (3.196) is the most general *ab initio* S matrix formulation of ATI including resonant ionization (ionization through intermediate atomic bound states). We restrict considerations only to nonresonant ionization so that

$$e^{-\imath \int^t d\tau V_L(\tau)} G_A^{(+)} e^{\imath \int^t d\tau V_L(\tau)} \approx G_L^{(+)} \quad (3.197)$$

Since

$$e^{-\imath \int^t d\tau V_L(\tau)} W(\vec{\alpha}) e^{\imath \int^t d\tau V_L(\tau)} = -W(-\vec{\alpha}) \quad (3.198)$$

and setting $\tau = t - t'$ we obtain

$$\begin{aligned} (S - 1)_{\text{fi}} &\approx -\imath \int_{-\infty}^\infty dt \langle e^{-\imath \int^t dt' V_L(t')} \Psi_{A, \vec{k}}^{(-)} | V_L \phi_i \rangle \\ &\quad - \imath \int_{-\infty}^\infty dt \int_0^\infty d\tau \langle e^{-\imath \int^t dt' V_L(t')} \Psi_{A, \vec{k}}^{(-)} | -W(-\vec{\alpha}) G_L^{(+)}(t, t - \tau) V_L(t - \tau) | \phi_i(t - \tau) \rangle \end{aligned} \quad (3.199)$$

denoting $S_{\text{fi}}^{(0)}$ to be the direct scattering term

$$S_{\text{fi}}^{(0)} = -i \int_{-\infty}^{\infty} dt \langle e^{-i \int^t dt' V_L(t')} \Psi_{A,\vec{k}}^{(-)} | V_L \phi_i \rangle \quad (3.200)$$

and $S_{\text{fi}}^{(1)}$ to be the rescattering term

$$S_{\text{fi}}^{(1)} = -i \int_{-\infty}^{\infty} dt \int_0^{\infty} d\tau \langle e^{-i \int^t dt' V_L(t')} \Psi_{A,\vec{k}}^{(-)} | -W(-\vec{\alpha}) G_L^{(+)}(t, t - \tau) V_L(t - \tau) | \phi_i(t - \tau) \rangle \quad (3.201)$$

so that

$$(S - 1)_{\text{fi}} \approx S_{\text{fi}}^{(0)} + S_{\text{fi}}^{(1)} \quad (3.202)$$

Eq. (3.202) with Eqs. (3.200) and (3.201) represent the most generalized *ab initio* S matrix formulation of ATI including rescattering with the most accurate consideration of the Coulomb effects in the final state wave function.

To the lowest order in the time dependent short range interaction $W(\vec{\alpha})$ we have

$$\Psi_{\text{f}}^{(-)}(\vec{r}, t) \approx e^{-i \int^t dt' V_L(t')} \Psi_{A,\vec{k}}^{(-)}(\vec{r}, t) \quad (3.203)$$

$$\approx e^{-i \int^t dt' \frac{A(t')^2}{2c^2}} \Psi_{A,\vec{k}}^{(-)}(\vec{r} - \vec{\alpha}(t), t) \quad (3.204)$$

where $\Psi_{A,\vec{k}}^{(-)}(\vec{r}, t)$ is given by

$$\Psi_{A,\vec{k}}^{(-)}(\vec{r}, t) = \frac{e^{\pi a/2} \Gamma(1 + ia)}{(2\pi)^{\frac{3}{2}}} {}_1F_1[-ia, 1, -i(kr + \vec{k} \cdot \vec{r})] e^{i\vec{k} \cdot \vec{r} - iE_k t} \quad (3.205)$$

$\Psi_{\text{f}}^{(-)}(\vec{r}, t)$ as given by Eq. (3.203) represents the most accurate consideration of the Coulomb effects in the ionization process. In section (3.4) we test this wave function, by showing that only this wave function and not the other wave functions commonly utilized in the literature (Volkov, Coulomb-Volkov and the most improved Coulomb-Volkov) satisfies the angular momentum considerations in the ionization process by circularly polarized electromagnetic field. In the following subsections a detailed evaluation of the generalized *ab initio* direct term $S_{\text{fi}}^{(0)}$, and the generalized *an initio* rescattering term $S_{\text{fi}}^{(1)}$ is presented.

3.3.1 Evaluation of the Generalized *ab initio* Direct Term

We start by writing

$$\Psi_{A,\vec{k}}(\vec{r}) = \frac{1}{(2\pi)^{\frac{3}{2}}} \int d\vec{q} e^{i\vec{q} \cdot \vec{r}} \tilde{\Psi}_{A,\vec{k}}(\vec{q}) \quad (3.206)$$

$$\phi_i(\vec{r}) = \frac{1}{(2\pi)^{\frac{3}{2}}} \int d\vec{q} e^{i\vec{q}\cdot\vec{r}} \tilde{\phi}_i(\vec{q}) \quad (3.207)$$

where $\tilde{\Psi}_{\Lambda,\vec{k}}(\vec{q})$ and $\tilde{\phi}_i(\vec{q})$ are the fourier transforms of $\Psi_{\Lambda,\vec{k}}(\vec{r})$ and $\phi_i(\vec{r})$ respectively

$$\tilde{\Psi}_{\Lambda,\vec{k}}(\vec{q}) = \frac{1}{(2\pi)^{\frac{3}{2}}} \int d\vec{r} e^{-i\vec{q}\cdot\vec{r}} \Psi_{\Lambda,\vec{k}}(\vec{r}) \quad (3.208)$$

$$= \frac{1}{(2\pi)^{\frac{3}{2}}} \int d\vec{r} e^{-i\vec{q}\cdot\vec{r}} \phi_i(\vec{r}) \quad (3.209)$$

Since

$$e^{-i \int^t dt' V_L(t')} e^{i\vec{q}\cdot\vec{r}} = e^{-i \int^t dt' V_L(\vec{q},t')} e^{i\vec{q}\cdot\vec{r}} \quad (3.210)$$

$$V_L e^{i\vec{q}\cdot\vec{r}} = V_L(\vec{q}) e^{i\vec{q}\cdot\vec{r}} \quad (3.211)$$

then the direct term reads

$$\begin{aligned} S_{\text{fi}}^{(0)} &= \left(\frac{1}{(2\pi)^3} \right) -i \int_{-\infty}^{\infty} dt \int d\vec{q} \int d\vec{q}' \int d\vec{r} e^{i(E_k + E_B)t} \tilde{\Psi}_{\Lambda,\vec{k}}^*(\vec{q}) e^{i \int^t dt' V_L(\vec{q},t')} e^{-i\vec{q}\cdot\vec{r}} \\ &\times \tilde{\phi}_i(\vec{q}') V_L(\vec{q}') e^{i\vec{q}'\cdot\vec{r}} \end{aligned} \quad (3.212)$$

The space integration yields a Dirac delta function $\delta(\vec{q} - \vec{q}')$, thus we have

$$S_{\text{fi}}^{(0)} = -i \int_{-\infty}^{\infty} dt \int d\vec{q} e^{i(E_k + E_B)t} \tilde{\Psi}_{\Lambda,\vec{k}}^*(\vec{q}) e^{i \int^t dt' V_L(\vec{q},t')} \tilde{\phi}_i(\vec{q}) V_L(\vec{q}) \quad (3.213)$$

The temporal integral is carried out by parts yielding

$$S_{\text{fi}}^{(0)} = (E_k + E_B) i \int_{-\infty}^{\infty} dt \int d\vec{q} e^{i(E_k + E_B)t} e^{i \int^t dt' V_L(\vec{q})} \tilde{\Psi}_{\Lambda,\vec{k}}^*(\vec{q}) \tilde{\phi}_i(\vec{q}) \quad (3.214)$$

Writing

$$e^{i \int^t dt' V_L(\vec{q})} = e^{i(U_{\text{p}}t + U_1(t) + \vec{q}\cdot\vec{\alpha})} \quad (3.215)$$

where

$$U(t) = \frac{1}{2c^2} \int^t dt' A^2(t') = U_{\text{p}}t + U_1(t) \quad (3.216)$$

we obtain

$$S_{\text{fi}}^{(0)} = (E_k + E_B) i \int_{-\infty}^{\infty} dt e^{i[(E_k + E_B + U_{\text{p}})t + U_1(t)]} \int d\vec{q} \tilde{\Psi}_{\Lambda,\vec{k}}^*(\vec{q}) \tilde{\phi}_i(\vec{q}) e^{i\vec{q}\cdot\vec{\alpha}} \quad (3.217)$$

Now,

$$\tilde{\Psi}_{A,\vec{k}}^*(\vec{q}) = \langle \vec{q} | \Psi_{A,\vec{k}}^{(-)*} \rangle = \frac{\Gamma(1-\imath a)e^{\pi a/2}}{(2\pi)^3} - \lim_{\lambda \rightarrow 0} \frac{\partial}{\partial \lambda} \int d\vec{r} e^{\imath(\vec{k}-\vec{q})\cdot\vec{r}} \frac{e^{-\lambda r}}{r} {}_1F_1[\imath a, 1, \imath(kr + \vec{k} \cdot \vec{r})] \quad (3.218)$$

This is a Nordsieck type integral which we evaluated earlier in Eq. (3.119) as J . Thus we have

$$\tilde{\Psi}_{A,\vec{k}}^*(\vec{q}) = \langle \vec{q} | \Psi_{A,\vec{k}}^{(-)*} \rangle = \frac{\Gamma(1-\imath a)e^{\pi a/2}}{2\pi^2} - \lim_{\lambda \rightarrow 0} \frac{\partial}{\partial \lambda} \frac{1}{(\vec{k} - \vec{q})^2 + \lambda^2} \left[\frac{q^2 - (k - \imath\lambda)^2}{(\vec{k} - \vec{q})^2 + \lambda^2} \right]^{-\imath a} \quad (3.219)$$

substituting back into Eq. (3.217) yields

$$\begin{aligned} S_{\text{fi}}^{(0)} &= \imath \frac{\Gamma(1-\imath a)e^{\pi a/2}}{2\pi^2} (E_k + E_B) \int_{-\infty}^{\infty} dt e^{\imath[(E_k + E_B + U_p)t + U_1(t)]} \\ &\times \int d\vec{q} \lim_{\lambda \rightarrow 0} -\frac{\partial}{\partial \lambda} \frac{1}{(\vec{k} - \vec{q})^2 + \lambda^2} \left[\frac{q^2 - (k - \imath\lambda)^2}{(\vec{k} - \vec{q})^2 + \lambda^2} \right]^{-\imath a} \tilde{\phi}_i(\vec{q}) e^{\imath\vec{q}\cdot\vec{\alpha}} \end{aligned} \quad (3.220)$$

the value of the integral in Eq. (3.220) is largely determined by the poles of the integrand. The poles are $q = k + \imath\lambda$ and $q = \imath Z$ which is due to $\tilde{\phi}_i(\vec{q})$. Moreover, due to the damping of the $e^{\imath\vec{q}\cdot\vec{\alpha}}$ term in the integral, the contribution due to the pole $q = k + \imath\lambda$ is larger than the pole $q = \imath Z$. Furthermore, if we carry the process of differentiation with respect to λ we will get a leading term which identified as a Dirac-delta function, namely

$$\lim_{\lambda \rightarrow 0} \frac{1}{\pi^2} \frac{\lambda}{[(\vec{k} - \vec{q})^2 + \lambda^2]^2} = \delta(\vec{q} - \vec{k}) \quad (3.221)$$

therefore, the value of the above integral is largely due to the pole $\vec{q} = \vec{k}$ and $\tilde{\phi}_i(\vec{q})$ is taken outside the integral and evaluated at $\vec{q} = \vec{k}$. Therefore, Eq. (3.220) now reads,

$$\begin{aligned} S_{\text{fi}}^{(0)} &\approx \imath \frac{\Gamma(1-\imath a)e^{\pi a/2}}{2\pi^2} (E_k + E_B) \int_{-\infty}^{\infty} dt e^{\imath[(E_k + E_B + U_p)t + U_1(t)]} \tilde{\phi}_i(\vec{k}) \\ &\times \int d\vec{q} \lim_{\lambda \rightarrow 0} -\frac{\partial}{\partial \lambda} \frac{1}{(\vec{k} - \vec{q})^2 + \lambda^2} \left[\frac{q^2 - (k - \imath\lambda)^2}{(\vec{k} - \vec{q})^2 + \lambda^2} \right]^{-\imath a} e^{\imath\vec{q}\cdot\vec{\alpha}} \end{aligned} \quad (3.222)$$

Utilizing Eq. (3.219) we obtain

$$S_{\text{fi}}^{(0)} \approx \imath (2\pi)^{\frac{3}{2}} (E_k + E_B) \int_{-\infty}^{\infty} dt e^{\imath[(E_k + E_B + U_p)t + U_1(t)]} \tilde{\phi}_i(\vec{k}) \frac{1}{(2\pi)^{\frac{3}{2}}} \int d\vec{q} \tilde{\Psi}_{A,\vec{k}}^*(\vec{q}) e^{\imath\vec{q}\cdot\vec{\alpha}} \quad (3.223)$$

comparing the integral

$$\frac{1}{(2\pi)^{\frac{3}{2}}} \int d\vec{q} \tilde{\Psi}_{A,\vec{k}}^*(\vec{q}) e^{i\vec{q}\cdot\vec{\alpha}}$$

with the Eq. (3.206)

$$\Psi_{A,\vec{k}}^{(-)}(\vec{r}) = \frac{1}{(2\pi)^{\frac{3}{2}}} \int d\vec{q} e^{i\vec{q}\cdot\vec{r}} \tilde{\Psi}_{A,\vec{k}}(\vec{q})$$

then it is obvious that

$$\frac{1}{(2\pi)^{\frac{3}{2}}} \int d\vec{q} \tilde{\Psi}_{A,\vec{k}}^*(\vec{q}) e^{i\vec{q}\cdot\vec{\alpha}} = \Psi_{A,\vec{k}}^{(-)*}(-\vec{\alpha}) = \Psi_{A,\vec{k}}^{(-)}(\vec{\alpha}) \quad (3.224)$$

Hence

$$S_{\text{fi}}^{(0)} \approx i(2\pi)^{\frac{3}{2}} (E_k + E_B) \int_{-\infty}^{\infty} dt e^{i[(E_k + E_B + U_p)t + U_1(t)]} \tilde{\phi}_i(\vec{k}) \Psi_{A,\vec{k}}^{(-)}(\vec{\alpha}) \quad (3.225)$$

$$\begin{aligned} &\approx i\Gamma(1 + ia) e^{\pi a/2} \langle \vec{k} | \phi_i \rangle (E_k + E_B) \\ &\times \int_{-\infty}^{\infty} dt e^{i[(E_k + E_B + U_p)t + U_1(t)]} e^{i\vec{k}\cdot\vec{\alpha}} {}_1F_1[-ia, 1, -i(k\alpha + \vec{k} \cdot \vec{\alpha})] \end{aligned} \quad (3.226)$$

The temporal integrand is periodic with period $2\pi/w$ and therefore we can write

$$S_{\text{fi}}^{(0)} \approx -2\pi i \sum_{n=n_0}^{\infty} \delta(E_k + E_B + U_p - nw) T_{\text{fi}}^{(0)}(n) \quad (3.227)$$

with

$$\begin{aligned} T_{\text{fi}}^{(0)}(n) &= -\Gamma(1 + ia) e^{\pi a/2} \langle \vec{k} | \phi_i \rangle (E_k + E_B) \\ &\times \frac{1}{2\pi} \int_0^{2\pi} d\varphi e^{i[\vec{k}\cdot\vec{\alpha} + U_1(\varphi) + n\varphi]} {}_1F_1[-ia, 1, -i\{k\alpha(\varphi) + \vec{k} \cdot \vec{\alpha}(\varphi)\}] \end{aligned} \quad (3.228)$$

where $\varphi = wt$.

3.3.2 Evaluation of the Generalized *ab initio* Rescattering Term

Recall the rescattering term, $S_{\text{fi}}^{(1)}$, is given by

$$S_{\text{fi}}^{(1)} = -i \int_{-\infty}^{\infty} dt \int_0^{\infty} d\tau \langle e^{-i\int^t dt' V_L(t')} \Psi_{A,\vec{k}}^{(-)} | -W(-\vec{\alpha}) G_L^{(+)}(t, t - \tau) V_L(t - \tau) | \phi_i(t - \tau) \rangle \quad (3.229)$$

The retarded Green's function, $G_L^{(+)}$, is given by

$$G_L^{(+)}(t, t - \tau) = -i\delta(\tau) \int d\vec{q} |\vec{q}\rangle \langle \vec{q}| e^{-iS(\vec{q}, t, \tau)} e^{-\eta\tau} \quad (3.230)$$

where $\eta \rightarrow 0^+$ is implied by the outgoing boundary conditions. $S(\vec{q}, t, \tau)$ is the semiclassical action for the propagation of an electron in the electromagnetic field from the moment of birth at $t - \tau$ to the moment of rescattering at t

$$S(\vec{q}, t, \tau) = \frac{1}{2} \int_{t-\tau}^t dt' [\vec{q} + \frac{\vec{A}}{c}]^2 \quad (3.231)$$

Substituting for $G^{(+)}$ and using the fact that the eigenstates of the free particle Hamiltonian form a complete set we obtain

$$\begin{aligned} S_{\text{fi}}^{(1)} &= -i \int_{-\infty}^{\infty} dt \int_0^{\infty} d\tau \int d\vec{q}' d\vec{q} \langle e^{-i \int^t dt' V_L(t')} \Psi_{A, \vec{k}}^{(-)} | \vec{q}' \rangle \langle \vec{q}' | -W(-\vec{\alpha}) | \vec{q} \rangle \\ &\times (-i) \langle \vec{q} | V_L(t - \tau) | \phi_i(t - \tau) \rangle e^{-iS(\vec{q}, t, \tau)} e^{-\eta\tau} \end{aligned} \quad (3.232)$$

since, V_L is a Hermitian operator we have

$$\begin{aligned} S_{\text{fi}}^{(1)} &= -i \int_{-\infty}^{\infty} dt \int_0^{\infty} d\tau \int d\vec{q}' d\vec{q} \langle e^{-i \int^t dt' V_L(\vec{q}', t')} \Psi_{A, \vec{k}}^{(-)} | \vec{q}' \rangle \langle \vec{q}' | -W(-\vec{\alpha}) | \vec{q} \rangle \\ &\times (-i) \langle \vec{q} | V_L(\vec{q}, t - \tau) | \phi_i(t - \tau) \rangle e^{-iS(\vec{q}, t, \tau)} e^{-\eta\tau} \end{aligned} \quad (3.233)$$

Now, the integral over \vec{q} is evaluated analytically using the saddle-point method [Appendix B] to obtain

$$\begin{aligned} S_{\text{fi}}^{(1)} &= -i \int_{-\infty}^{\infty} dt \int_0^{\infty} d\tau \int d\vec{q}' \langle e^{-i \int^t dt' V_L(\vec{q}', t')} \Psi_{A, \vec{k}}^{(-)} | \vec{q}' \rangle \langle \vec{q}' | -W(-\vec{\alpha}) | \vec{q}_s \rangle \\ &\times (-i) \langle \vec{q}_s | V_L(\vec{q}_s, t - \tau) | \phi_i(t - \tau) \rangle e^{-iS(\vec{q}_s, t, \tau)} e^{-\eta\tau} \left(\frac{2\pi}{i\tau + \epsilon} \right)^{\frac{3}{2}} \end{aligned} \quad (3.234)$$

where

$$\vec{q}_s = \frac{1}{\tau} [\vec{\alpha}(t - \tau) - \vec{\alpha}(t)] \quad (3.235)$$

is the solution of $\vec{\nabla}_{\vec{q}} S(\vec{q}, t, \tau) = 0$, and the parameter ϵ is introduced to smooth the singularity in τ . Now,

$$W(-\vec{\alpha}) = V_A(\vec{r} - \vec{\alpha}) - V_A(\vec{r}) \quad (3.236)$$

so we have

$$\langle \vec{q}' | -W(-\vec{\alpha}) | \vec{q}_s \rangle = \frac{Z}{2\pi^2} \frac{[e^{-\imath(\vec{q}' - \vec{q}_s) \cdot \vec{\alpha}} - 1]}{|\vec{q}' - \vec{q}_s|^2} \quad (3.237)$$

It is to be noticed that $\vec{q}' = \vec{q}_s$ occurs when $\vec{\alpha} = 0$ and therefore $\langle \vec{q}' | -W(-\vec{\alpha}) | \vec{q}_s \rangle = 0$ when $\vec{q}' = \vec{q}_s$ and so it is singularity free. It is a fortification of the the fact that the high energy electrons are due to rescattering by the short range potential $W(\vec{\alpha})$ which allows only the off shell essential state resonances to be populated signifying the continuum-continuum transitions.

Now, to evaluate the integral over \vec{q}' we write

$$\begin{aligned} S_{\text{fi}}^{(1)} &= -\imath \int_{-\infty}^{\infty} dt \int_0^{\infty} d\tau \left(\frac{2\pi}{\imath\tau + \epsilon} \right)^{\frac{3}{2}} e^{\imath[E_k t + U_p t + U_1(t) + E_B(t - \tau)]} e^{-\imath S(\vec{q}_s, t, \tau)} e^{-\eta\tau} \langle \vec{q}_s | \phi_i \rangle \\ &\times V_L(\vec{q}_s, t - \tau) (-\imath) \int d\vec{q}' e^{\imath\vec{q}' \cdot \vec{\alpha}} \langle \Psi_{A, \vec{k}}^{(-)} | \vec{q}' \rangle \langle \vec{q}' | -W(-\vec{\alpha}) | \vec{q}_s \rangle \end{aligned} \quad (3.238)$$

the value of the integral over \vec{q}' is mainly determined by the poles of the integrand; i.e., the poles of $\langle \vec{q}' | -W(-\vec{\alpha}) | \vec{q}_s \rangle$ at $\vec{q}' = \vec{q}_s$ and the poles of $\langle \Psi_{A, \vec{k}}^{(-)} | \vec{q}' \rangle$ at $\vec{q}' = \vec{k}$. As we discussed previously the pole at $\vec{q}' = \vec{k}$ give rise to a Dirac delta function $\delta(\vec{q}' - \vec{k})$ and from Eq. (2.37) it is justifiable to assume that the value of the integral is largely determined by the poles of $\langle \Psi_{A, \vec{k}}^{(-)} | \vec{q}' \rangle$ at $\vec{q}' = \vec{k}$ and so $\langle \vec{q}' | -W(-\vec{\alpha}) | \vec{q}_s \rangle$ may be taken outside the integral sign and evaluated at $\vec{q}' = \vec{k}$. Thus, as we did previously, the value of the integral over \vec{q}' equals $(2\pi)^{\frac{3}{2}} \langle \vec{k} | -W(-\vec{\alpha}) | \vec{q}_s \rangle \Psi_{A, \vec{k}}^{(-)}(\vec{r} = \vec{\alpha})$. Taking this into account, we obtain

$$\begin{aligned} S_{\text{fi}}^{(1)} &\approx -\imath \int_{-\infty}^{\infty} dt \int_0^{\infty} d\tau \left(\frac{2\pi}{\imath\tau + \epsilon} \right)^{\frac{3}{2}} e^{\imath[E_k t + U_p t + U_1(t) + E_B(t - \tau)]} e^{-\imath S(\vec{q}_s, t, \tau)} e^{-\eta\tau} \langle \vec{q}_s | \phi_i \rangle \\ &\times V_L(\vec{q}_s, t - \tau) (-\imath) (2\pi)^{\frac{3}{2}} \langle \vec{k} | -W(-\vec{\alpha}) | \vec{q}_s \rangle \Psi_{A, \vec{k}}^{(-)}(\vec{r} = \vec{\alpha}) \end{aligned} \quad (3.239)$$

Since

$$S(\vec{q}_s, t, \tau) = -\frac{1}{2} q_s^2 \tau + U_p \tau + U_1(t) - U_1(t - \tau) \quad (3.240)$$

and

$$\Psi_{A, \vec{k}}^{(-)}(\vec{\alpha}) = \frac{\Gamma(1 + \imath a) e^{\pi a/2}}{(2\pi)^{\frac{3}{2}}} e^{\imath \vec{k} \cdot \vec{\alpha}} {}_1F_1[-\imath a, 1, -\imath(k\alpha + \vec{k} \cdot \vec{\alpha})] \quad (3.241)$$

then using Eqs. (3.237) we obtain

$$S_{\text{fi}}^{(1)} \approx -\imath \frac{Z \Gamma(1 + \imath a) e^{\pi a/2}}{2\pi^2} \int_{-\infty}^{\infty} dt \int_0^{\infty} d\tau \left(\frac{2\pi}{\imath\tau + \epsilon} \right)^{\frac{3}{2}} e^{\imath[E_k t + U_p t + E_B t]}$$

$$\begin{aligned}
& \times e^{i[\frac{1}{2}q_s^2\tau + U_1(t-\tau) - (E_B + U_p)\tau]} e^{-\eta\tau} (-i) \langle \vec{q}_s | \phi_i \rangle V_L(\vec{q}_s, t - \tau) \frac{[e^{-i(\vec{k} - \vec{q}_s) \cdot \vec{\alpha}} - 1]}{|\vec{k} - \vec{q}_s|^2} \\
& \times e^{i\vec{k} \cdot \vec{\alpha}} {}_1F_1[-ia, 1, -i(k\alpha + \vec{k} \cdot \vec{\alpha})]
\end{aligned} \tag{3.242}$$

The temporal integrand is periodic with period $2\pi/w$ and therefore we can write

$$S_{\text{fi}}^{(1)} \approx -2\pi i \sum_{n=n_0}^{\infty} \delta(E_k + E_B + U_p - nw) T_{\text{fi}}^{(1)}(n) \tag{3.243}$$

with

$$\begin{aligned}
T_{\text{fi}}^{(1)}(n) &= -i \frac{Z \Gamma(1 + ia) e^{\pi a/2}}{2\pi^2} \frac{1}{2\pi} \int_0^{2\pi} d\varphi e^{i[\vec{k} \cdot \vec{\alpha}(\varphi) + n\varphi]} {}_1F_1[-ia, 1, -i\{k\alpha(\varphi) + \vec{k} \cdot \vec{\alpha}(\varphi)\}] \\
&\times \int_0^{\infty} d\tau \left(\frac{2\pi}{i\tau + \epsilon} \right)^{\frac{3}{2}} \langle \vec{q}_s | \phi_i \rangle V_L(\vec{q}_s, \varphi - \tau) \frac{[e^{-i(\vec{k} - \vec{q}_s) \cdot \vec{\alpha}(\varphi)} - 1]}{|\vec{k} - \vec{q}_s|^2} \\
&\times e^{i[\frac{1}{2}q_s^2\tau + U_1(t-\tau) - (E_B + U_p)\tau]} e^{-\eta\tau}
\end{aligned} \tag{3.244}$$

where $\varphi = wt$ and $q_s = q_s(\varphi, \tau)$. If we write

$$(S - 1)_{\text{fi}} \approx S_{\text{fi}}^{(0)} + S_{\text{fi}}^{(1)} = -2\pi i \sum_{n=n_0}^{\infty} \delta(E_k + E_B + U_p - nw) T_{\text{fi}}(n) \tag{3.245}$$

then the differential ionization rate, $w_{\text{fi}}(n, \theta)$, is

$$w_{\text{fi}} = 2\pi k_f(n) |T_{\text{fi}}(n)|^2 \tag{3.246}$$

where $k_f(n) = \sqrt{2(nw - U_p - E_B)}$ and

$$\begin{aligned}
T_{\text{fi}}(n) &= T_{\text{fi}}^{(0)}(n) + T_{\text{fi}}^{(1)}(n) \\
T_{\text{fi}}^{(0)}(n) &= -\Gamma(1 + ia) e^{\pi a/2} \langle \vec{k} | \phi_i \rangle (E_k + E_B) \frac{1}{2\pi} \int_0^{2\pi} d\varphi e^{i[\vec{k} \cdot \vec{\alpha} + U_1(\varphi) + n\varphi]} \\
&\times {}_1F_1[-ia, 1, -i\{k\alpha(\varphi) + \vec{k} \cdot \vec{\alpha}(\varphi)\}] \\
T_{\text{fi}}^{(1)}(n) &= -i \frac{Z \Gamma(1 + ia) e^{\pi a/2}}{2\pi^2} \frac{1}{2\pi} \int_0^{2\pi} d\varphi e^{i[\vec{k} \cdot \vec{\alpha}(\varphi) + n\varphi]} {}_1F_1[-ia, 1, -i\{k\alpha(\varphi) + \vec{k} \cdot \vec{\alpha}(\varphi)\}] \\
&\times \int_0^{\infty} d\tau \left(\frac{2\pi}{i\tau + \epsilon} \right)^{\frac{3}{2}} \langle \vec{q}_s | \phi_i \rangle V_L(\vec{q}_s, \varphi - \tau) \frac{[e^{-i(\vec{k} - \vec{q}_s) \cdot \vec{\alpha}(\varphi)} - 1]}{|\vec{k} - \vec{q}_s|^2} \\
&\times e^{i[\frac{1}{2}q_s^2\tau + U_1(t-\tau) - (E_B + U_p)\tau]} e^{-\eta\tau}
\end{aligned} \tag{3.247}$$

Eqs. (3.246) and (3.247) represent the most generalized *ab initio* S matrix formulation for above threshold ionization including rescattering with the most accurate considerations of Coulomb effects to all orders.

3.4 The Final State Wave Function

As a consequence of the *ab initio* formulation of above threshold ionization, we deduced that the long-range Coulomb potential affects the low energy photoelectrons. Recent experimental findings [73-75,78-79] and numerical solutions of the time dependent Schrödinger equation [76-77,80-81] confirm the importance of the long-range Coulomb potential on the low energy photoelectrons. Thus it is imperative to improve the final state wave function by accurately including Coulomb effects in the final state wave function.

In a recent experiment by Eckle et al. (2009) [60], published in the journal Science, the photoelectron momentum distributions show counter-intuitive shifts. They irradiated helium atoms with circularly polarized femtosecond pulses with parameters suitable for the tunneling regime and invoked the concept of tunneling time to explain the shift. Aware of the experiment, Martiny et al. [61] solved the three dimensional Schrödinger equation for a short circularly polarized pulse interacting with hydrogen atom. The photoelectron momentum distributions show counter-intuitive shifts (see Fig. 3.1), similar to those observed by Eckle et al. [60]. Furthermore, the Martiny et al. [61] calculation show these shifts in the multiphoton regime. They explained the shifts in terms of angular momentum considerations. The shifts are a manifestation of the fact that $\langle \Psi | L_z | \Psi \rangle = \langle L_z \rangle \neq 0$ after the pulse, which implies that the azimuthal velocity is non-vanishing, which in turn, makes the distribution rotates compared to the $\langle L_z \rangle = 0$ case. The hydrogen atom is initially in the ground state and hence, $\langle L_z \rangle = 0$, before the pulse. According to Ehrenfest's theorem,

$$\frac{d}{dt} \langle L_z \rangle = i \langle [H, L_z] \rangle \quad (3.248)$$

which forces the liberated electron to pick up a nonzero value of $\langle L_z \rangle$, since $[H, L_z] \neq 0$ during the pulse for $H = H_0 + \vec{A} \cdot \vec{P} + \frac{A^2}{2}$, H_0 being the free Hamiltonian. The mean value of L_z changes during the pulse, in accordance with Ehrenfest's theorem, until it becomes a constant with the value

$$\langle L_z \rangle = i \int_0^T \langle [H, L_z] \rangle dt \quad (3.249)$$

after the pulse. Although $[H, L_z] \neq 0$, it remains true that, $\langle [H, L_z] \rangle = 0$ for a Volkov state. Moreover, Martiny et al. [61] calculations using the Coulomb-Volkov wave function show

little or no shift. In circular polarization ionization, there are N units of angular momentum transferred during ionization, where N is the number of absorbed photons. Martiny et al. [61] suggest that an accurate considerations of Coulomb effects in the final state wave function will produce such shifts which are a manifestation of N units of angular momentum being transferred during ionization. Aware of this, we will show that the wave function which we introduced above and given by Eq. (3.205) preserves angular momentum considerations, and therefore should produce such shifts. This equation provides an accurate account of Coulomb effects in the final state wave function.

Accurate considerations of Coulomb effects in the final state have to be taken into account in order to interpret the recent experimental findings in above threshold ionization (ATI) by a linearly polarized light. The low energy momentum distributions reported by Moshhammer et al. [73], Rudenko et al. [74] (see Fig. 3.2), and Mahrajan et al. [75] showed features that can not be explained within the strong field approximation (SFA). The numerical calculations of Chen et al. [76], and Guo et al. [77] confirmed the role of Coulomb effects in the low energy momentum distributions. Furthermore, Blaga et al. [78], and Quan et al. [79] have recently presented a high resolution photoelectron energy spectra that manifests an unexpected characteristic spike-like structure at low energy, which becomes prominent at midinfrared wavelength ($\lambda > 1\mu m$) (see Fig. 3.3). These structures can not be explained within the strong field approximation (SFA). Recently, theoretical calculation of Yan et al. [80] in which simple inclusion of the Coulomb effects in the quantum orbits revealed such structures.

From the above discussion it is imperative to carefully examine the transition amplitude given by Eq. (3.228). This is because the transition amplitude as given by Eq. (3.228) provides an accurate account of Coulomb effects in the final state wave function.

We recall the final state wave function $\Psi_f^{(-)}$ is given by Eq. (3.205)

$$\Psi_f^{(-)}(\vec{r}, t) \approx e^{-i \int^t dt' V_L(t')} \Psi_{A,k}^{(-)}(\vec{r}, t) \quad (3.250)$$

$$\approx e^{-i \int^t dt' \frac{A(t')^2}{2c^2}} \Psi_{A,k}^{(-)}(\vec{r} - \vec{\alpha}(t), t) \quad (3.251)$$

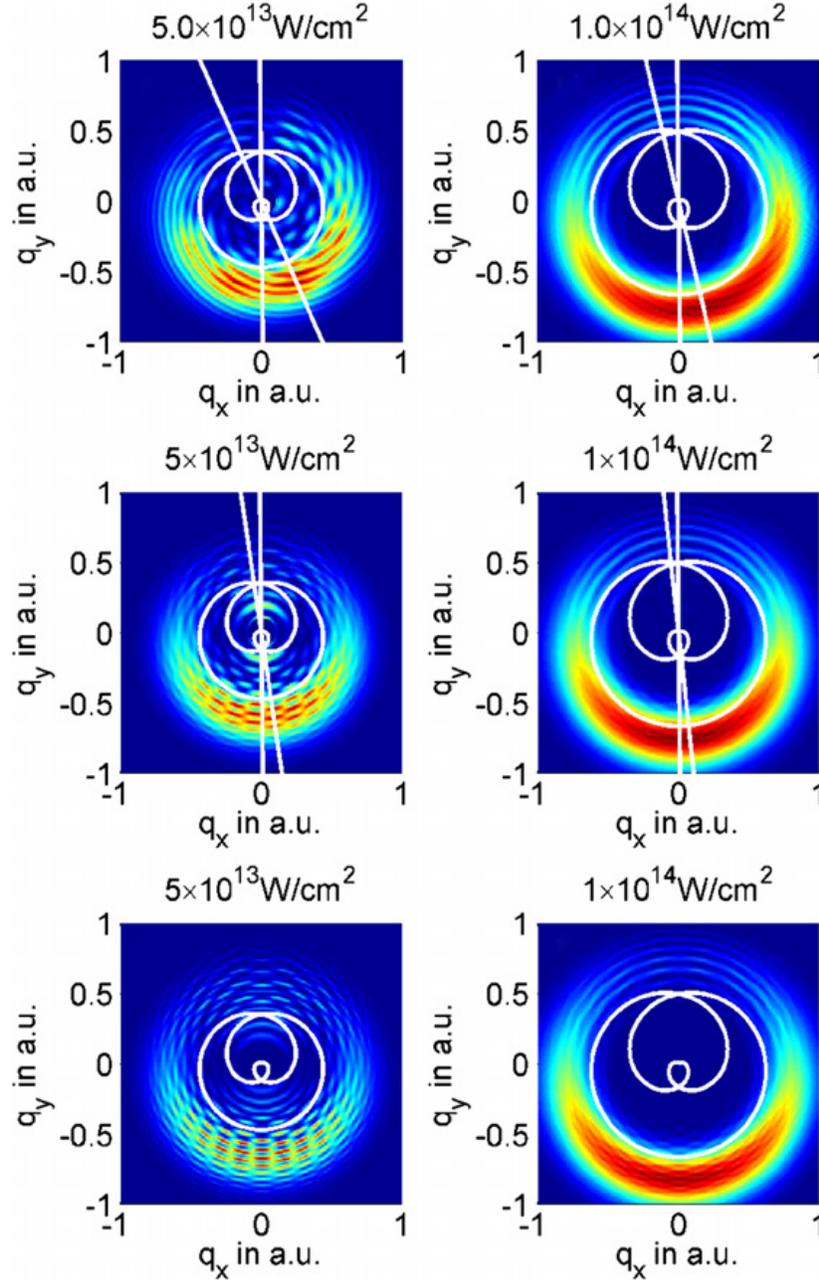


Figure 3.1: Momentum distributions in the plane of polarization for strong field ionization of H(1s) from Martiny et al. [61]. Panels (a) and (b) show results obtained by solving the TDSE; panels (c) and (d) show results obtained using the Coulomb Volkov corrected SFA, while panels (e) and (f) show results obtained using SFA. The curves show $-\vec{A}(t)$, while the straight lines in (a) and (b) highlight the angular shift. The laser wavelength is 800 nm.

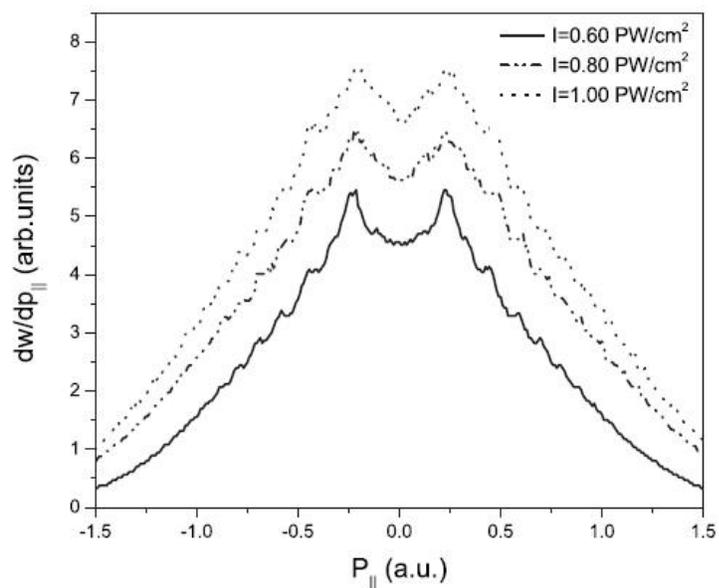


Figure 3.2: Experimental distributions of parallel momentum (along polarization direction) for He atom in an intense 25 fs, 795 nm laser pulse at three peak intensities: $I = .6 \text{ PW/cm}^2$, $I = .8 \text{ PW/cm}^2$, $I = 1.0 \text{ PW/cm}^2$. The experimental data are taken from Rudenko et al. [74]. Notice the central minimum and the double peak structure. The SFA predicts a central maximum.

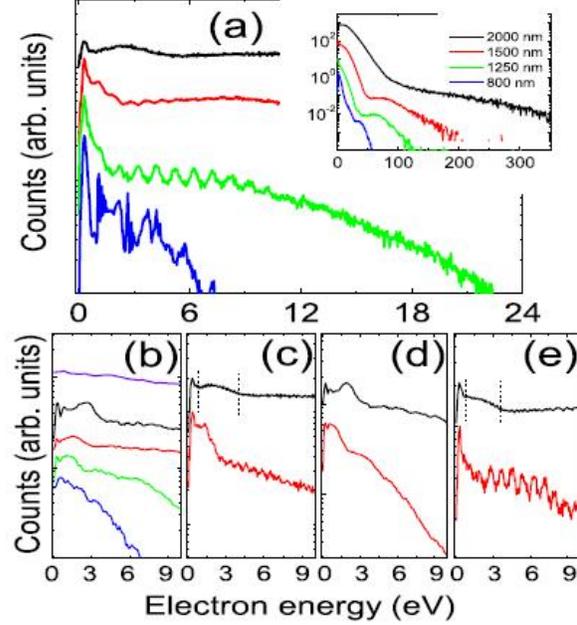


Figure 3.3: Experimental [(a), (c), and (e)] and calculated [(b), (d)] photoelectron spectra of Xenon from Quan et al. [79]. (a) $I = .08 \text{ PW/cm}^2$, $\lambda = 800, 1250, 1500,$ and 2000 nm from bottom to top, respectively. The complete spectra are shown in the inset. The laser pulse durations are 40 fs at 800 nm, 30 fs at 1250 nm, and 1500 nm, while 90 fs at 2000 nm. (b) $I = .08 \text{ PW/cm}^2$ and $\lambda = 800, 1250, 1500,$ and 2000 nm , with Coulomb potential for the curves from bottom to top, respectively. While the uppermost curves is for $I = .08 \text{ PW/cm}^2$ and $\lambda = 2000 \text{ nm}$ without Coulomb potential. (c), (d) $\lambda = 2000 \text{ nm}$, $I = .032, .064 \text{ PW/cm}^2$ for the lower and upper curves respectively. (e) $\lambda = .04, .1 \text{ PW/cm}^2$ for the lower and upper curves respectively. In (c), and (e) the boundaries of the second hump are indicated by the dashed lines for higher intensities.

where $\Psi_{A,\vec{k}}^{(-)}(\vec{r}, t)$ is given by

$$\Psi_{A,\vec{k}}^{(-)}(\vec{r}, t) = \frac{e^{\pi a/2} \Gamma(1 + ia)}{(2\pi)^{\frac{3}{2}}} {}_1F_1[-ia, 1, -i(kr + \vec{k} \cdot \vec{r})] e^{i\vec{k} \cdot \vec{r} - iE_k t} \quad (3.252)$$

The transition amplitude from the ground state ϕ_i to final continuum state $\Psi_f^{(-)}$ is

$$(S - 1)_{fi} = -i \int_{-\infty}^{\infty} dt \langle \Psi_f^{(-)} | V_L \phi_i \rangle \quad (3.253)$$

This amplitude was evaluated earlier resulting in Eqs. (3.227) and (3.228), namely

$$(S - 1)_{fi} = -2\pi i \sum_{n=n_o}^{\infty} \delta(E_k + U_p + E_B - nw) T_{fi}(n) \quad (3.254)$$

with

$$\begin{aligned} T_{fi}(n) &= -\Gamma(1 + ia) e^{\pi a/2} \langle \vec{k} | \phi_i \rangle (E_k + E_B) \frac{1}{2\pi} \int_0^{2\pi} d\varphi e^{i[\vec{k} \cdot \vec{\alpha} + U_1(\varphi) + n\varphi]} \\ &\times {}_1F_1[-ia, 1, -i\{k\alpha(\varphi) + \vec{k} \cdot \vec{\alpha}(\varphi)\}] \\ &= (2\pi)^{\frac{3}{2}} \langle \vec{k} | \phi_i \rangle (E_k + E_B) \frac{1}{2\pi} \int_0^{2\pi} d\varphi e^{i[U_1(\varphi) + n\varphi]} \Psi_{A,\vec{k}}^{(-)}(\vec{r} = \vec{\alpha}) \end{aligned} \quad (3.255)$$

where $\varphi = wt$.

Now, consider

$$\Psi_{A,\vec{k}}^{(-)}(\vec{r} = \vec{\alpha}) = N_a e^{i\vec{k} \cdot \vec{\alpha}} {}_1F_1[-ia, 1, -i\{k\alpha(\varphi) + \vec{k} \cdot \vec{\alpha}(\varphi)\}] \quad (3.256)$$

where

$$N_a = \frac{\Gamma(1 + ia) e^{\pi a/2}}{(2\pi)^{\frac{3}{2}}}$$

Using the integral representation of ${}_1F_1[\beta, \gamma, z]$ [71]

$${}_1F_1[\beta, \gamma, z] = \frac{\Gamma(\gamma)}{\Gamma(\beta)\Gamma(\gamma - \beta)} \int_0^1 ds e^{zs} s^{\beta-1} (1-s)^{\gamma-\beta-1} \quad (3.257)$$

then $\Psi_{A,\vec{k}}^{(-)}(\vec{\alpha})$ can be written as

$$\Psi_{A,\vec{k}}^{(-)}(\vec{\alpha}) = \frac{N_a}{\Gamma(-ia)\Gamma(1 + ia)} \int_0^1 ds e^{-ik\alpha s} e^{-i(s-1)\vec{k} \cdot \vec{\alpha}} s^{-ia-1} (1-s)^{ia} \quad (3.258)$$

Let ϑ is the angle between \vec{k} and $\vec{\alpha}$. Using the partial wave expansion

$$e^{-i\vec{k} \cdot \vec{\alpha}} = \sum_{l=0}^{\infty} (2l+1)(-i)^l j_l(k\alpha) P_l(\cos \vartheta) \quad (3.259)$$

then we have

$$\Psi_{A,\vec{k}}^{(-)}(\vec{\alpha}) = \frac{N_a}{\Gamma(-ia)\Gamma(1+ia)} \sum_{l=0}^{\infty} (2l+1)(-i)^l P_l(\cos \vartheta) \int_0^1 ds e^{-ik\alpha s} j_l[(s-1)k\alpha] s^{-ia-1}(1-s)^{ia} \quad (3.260)$$

Using the series representation of ${}_1F_1[\beta, \gamma, z]$ [71]

$${}_1F_1[\beta, \gamma, z] = \sum_{p=0}^{\infty} \frac{\Gamma(\beta+p)\Gamma(\gamma)}{\Gamma(\beta)\Gamma(\gamma+p)} \frac{z^p}{p!} \quad (3.261)$$

and since

$$j_l(z) = \frac{2^l l!}{(2l+1)!} z^l e^{iz} {}_1F_1[l+1, 2l+1, -2iz] \quad (3.262)$$

then

$$j_l[(s-1)k\alpha] = 2^l (k\alpha)^l (s-1)^l e^{is k\alpha} e^{-ik\alpha} \sum_{p=0}^{\infty} \frac{(l+p)!}{(2l+1+p)!} (s-1)^p \frac{(-2ik\alpha)^p}{p!} \quad (3.263)$$

and therefore we obtain

$$\begin{aligned} \Psi_{A,\vec{k}}^{(-)}(\vec{\alpha}) &= \frac{N_a}{\Gamma(-ia)\Gamma(1+ia)} \sum_{l=0}^{\infty} (2l+1)(-i)^l P_l(\cos \vartheta) (2k\alpha)^l e^{-ik\alpha} \sum_{p=0}^{\infty} \frac{(l+p)!}{(2l+1+p)!} (-1)^{l+p} \\ &\times \left\{ \int_0^1 ds s^{-ia-1} (1-s)^{l+p+ia} \right\} \frac{(-2ik\alpha)^p}{p!} \end{aligned} \quad (3.264)$$

Now, the beta function $B(x, y)$ is defined as [71]

$$B(x, y) = \frac{\Gamma(x)\Gamma(y)}{\Gamma(x+y)} = \int_0^1 ds s^{x-1} (1-s)^{y-1} \quad (3.265)$$

and so we have

$$\begin{aligned} \Psi_{A,\vec{k}}^{(-)}(\vec{\alpha}) &= \frac{N_a \Gamma(-ia)}{\Gamma(-ia)\Gamma(1+ia)} \sum_{l=0}^{\infty} (2l+1)(i)^l P_l(\cos \vartheta) (2k\alpha)^l e^{-ik\alpha} \\ &\times \sum_{p=0}^{\infty} \frac{\Gamma(l+p+1+ia)}{\Gamma(2l+2+p)} \frac{(-2ik\alpha)^p}{p!} \\ &= \frac{N_a \Gamma(-ia)}{\Gamma(-ia)\Gamma(1+ia)} \sum_{l=0}^{\infty} (2l+1)(i)^l P_l(\cos \vartheta) (2k\alpha)^l e^{-ik\alpha} \\ &\times \frac{\Gamma(l+1+ia)}{\Gamma(2l+2)} {}_1F_1[l+1+ia, 2l+2, 2ik\alpha] \end{aligned} \quad (3.266)$$

since

$$\begin{aligned}\Gamma(l+1+\imath a) &= (l+\imath a)(l-1+\imath a)(l-2+\imath a)\cdots(1+\imath a)(\imath a)\Gamma(\imath a) \\ \Gamma(l+1-\imath a) &= (l-\imath a)(l-1-\imath a)(l-2-\imath a)\cdots(1-\imath a)(-\imath a)\Gamma(-\imath a) \\ \Gamma(1+z) &= z\Gamma(z) \\ \Gamma(z)\Gamma(1-z) &= \frac{\pi}{\sin \pi z}\end{aligned}$$

then

$$\Gamma(l+1+\imath a) = |\Gamma(l+1+\imath a)|e^{-\imath\delta_l} \quad (3.267)$$

$$= \sqrt{\frac{2\pi a e^{-a}}{1-e^{-2\pi a}}} \prod_{s=1}^l \sqrt{(s^2+a^2)} e^{-\imath\delta_l} \quad (3.268)$$

where δ_l is the argument of $\Gamma(l+1-\imath a)$. Substituting Eq. (3.268) into Eq. (3.266) and using the spherical harmonics addition theorem

$$P_l(\cos \vartheta) = \frac{4\pi}{2l+1} \sum_{m=-l}^l Y_l^m(\theta_\alpha, \phi_\alpha) Y_l^{m*}(\theta_k, \phi_k) \quad (3.269)$$

we arrive at

$$\begin{aligned}\Psi_{\mathbf{A},\mathbf{k}}^{(-)}(\vec{\alpha}) &= \frac{\sqrt{Z}}{\sqrt{2\pi k}} \sum_{l=0}^{\infty} \sum_{m=-l}^l i^l e^{-\imath\delta_l} \sqrt{\frac{8\pi}{a(1-e^{-2\pi a})}} \prod_{s=1}^l \sqrt{(s^2+a^2)} \frac{(2k\alpha)^l}{(2l+1)!} e^{-ik\alpha} \\ &\times {}_1F_1[l+1+\imath a, 2l+2, 2ik\alpha] Y_l^m(\theta_\alpha, \phi_\alpha) Y_l^{m*}(\theta_k, \phi_k)\end{aligned} \quad (3.270)$$

The significance of Eq. (3.270) is that it upholds angular momentum conservation in the ionization process as well as it allows a careful examination of the low energy photoelectron momentum and energy distributions. In the following subsections we look at Eq. (3.270) for both circularly and linearly polarized lights.

3.4.1 The Case of Circularly Polarized Light

For circularly polarized light propagating along the z -axis the vector potential \vec{A} is

$$\begin{aligned}\vec{A}(t) &= \frac{A_0}{\sqrt{2}}(\cos wt \hat{\mathbf{i}} + \sin wt \hat{\mathbf{j}}) \\ \vec{\alpha}(t) &= \frac{A_0}{\sqrt{2}cw}(\sin wt \hat{\mathbf{i}} - \cos wt \hat{\mathbf{j}}) = \frac{\sqrt{2U_p}}{w}(\sin wt \hat{\mathbf{i}} - \cos wt \hat{\mathbf{j}}) = \left(\frac{\sqrt{2U_p}}{w}, \pi/2, (2\pi - wt)\right) \\ U_1(t) &= 0\end{aligned}$$

and since

$$\begin{aligned} Y_l^m(\theta, \phi) &= (-)^m \left[\frac{(2l+1)(l-m)!}{4\pi(l+m)!} \right]^{\frac{1}{2}} P_l^m(\cos \theta) e^{im\phi} \\ Y_l^{-m}(\theta, \phi) &= (-)^m Y_l^{m*}(\theta, \phi) \end{aligned}$$

then we have

$$\begin{aligned} \Psi_{A, \vec{k}}^{(-)}(\vec{\alpha}) &= \frac{\sqrt{Z}}{\sqrt{2\pi k}} \sum_{l=0}^{\infty} \sum_{m=-l}^l i^l e^{-i\delta_l} \sqrt{\frac{8\pi}{a(1-e^{-2\pi a})}} \prod_{s=1}^l \sqrt{(s^2+a^2)} \frac{(2k \frac{\sqrt{2U_P}}{w})^l}{(2l+1)!} e^{-ik \frac{\sqrt{2U_P}}{w}} \\ &\times \left[\frac{(2l+1)(l-m)!}{4\pi(l+m)!} \right] {}_1F_1[l+1+ia, 2l+2, 2ik \frac{\sqrt{2U_P}}{w}] P_l^m(0) P_l^m(\cos \theta_k) e^{-im\varphi} e^{-im\phi_k} \end{aligned} \quad (3.271)$$

where $\varphi = wt$. Thus, Eq. (3.255) for the transition amplitude $T_{\text{fi}}(n)$ with the absorption of n photons now becomes

$$\begin{aligned} T_{\text{fi}}(n) &= \frac{\sqrt{Z}}{\sqrt{2\pi k}} \sum_{l=0}^{\infty} \sum_{m=-l}^l i^l e^{-i\delta_l} \sqrt{\frac{8\pi}{a(1-e^{-2\pi a})}} \prod_{s=1}^l \sqrt{(s^2+a^2)} \frac{(2k \frac{\sqrt{2U_P}}{w})^l}{(2l+1)!} e^{-ik \frac{\sqrt{2U_P}}{w}} \\ &\times \left[\frac{(2l+1)(l-m)!}{4\pi(l+m)!} \right] {}_1F_1[l+1+ia, 2l+2, 2ik \frac{\sqrt{2U_P}}{w}] P_l^m(0) P_l^m(\cos \theta_k) e^{-im\phi_k} \\ &\times (2\pi)^{\frac{3}{2}} \langle \vec{k} | \phi_i \rangle (E_k + E_B) \frac{1}{2\pi} \int_0^{2\pi} d\varphi e^{i(n-m)\varphi} \end{aligned} \quad (3.272)$$

Since

$$\frac{1}{2\pi} \int_0^{2\pi} d\varphi e^{i(n-m)\varphi} = \delta_{n,m}$$

we arrive at the conclusion that only the partial wave in which the magnetic quantum number m equals the number of absorbed photons n contribute to the transition. This means that the change in the z component of the angular momentum in the ionization process equals the number of absorbed photons. Moreover, since $P_l^m(0) \neq 0$ only if $l+m$ is an even integer, then we have $l+n$ is always even and so $T_{\text{fi}}(n)$ simplifies to

$$\begin{aligned} T_{\text{fi}}(n) &= \frac{\sqrt{Z}}{\sqrt{2\pi k}} \sum_{l=n}^* i^l e^{-i\delta_l} \sqrt{\frac{8\pi}{a(1-e^{-2\pi a})}} \prod_{s=1}^l \sqrt{(s^2+a^2)} \frac{(2k \frac{\sqrt{2U_P}}{w})^l}{(2l+1)!} e^{-ik \frac{\sqrt{2U_P}}{w}} \\ &\times \left[\frac{(2l+1)(l-n)!}{4\pi(l+n)!} \right] {}_1F_1[l+1+ia, 2l+2, 2ik \frac{\sqrt{2U_P}}{w}] P_l^n(0) P_l^n(\cos \theta_k) e^{-in\phi_k} \\ &\times (2\pi)^{\frac{3}{2}} \langle \vec{k} | \phi_i \rangle (E_k + E_B) \end{aligned} \quad (3.273)$$

and the asterisks * on the sum indicates only terms with $l + n$ even are included. It is to be noticed that when $2k\sqrt{2U_p}/lw \ll 1$, then contributions of higher values of l are negligible. Therefore we can terminate the sum in Eq. (2.73) at a cut-off value determined by the criterion $2k\sqrt{2U_p}/lw \ll 1$.

For laser parameters in which $n_0 \gg 1$ where n_0 , is the minimum number required for threshold ionization, then we can set $l + 1 + ia \approx l + 1$. Since

$${}_1F_1[\alpha, 2\alpha, z] = e^{\frac{z}{2}} \left(\frac{z}{4}\right)^{\frac{1}{2}-\alpha} \Gamma(\alpha + \frac{1}{2}) I_{\alpha-\frac{1}{2}}(z) \quad (3.274)$$

$$I_{\alpha-\frac{1}{2}}(z) = i^{-(\alpha-\frac{1}{2})} J_{\alpha-\frac{1}{2}}(iz) \quad (3.275)$$

$$j_l(z) = \sqrt{\pi/2z} J_{l+\frac{1}{2}}(z) \quad (3.276)$$

Then we have

$$\begin{aligned} T_{\text{fi}}(n) &= \frac{\sqrt{Z}}{\sqrt{2\pi k}} \sum_{l=n}^* \frac{i^{-l} 2^{2l+1}}{\sqrt{\pi}} \sqrt{\frac{8\pi}{a(1-e^{-2\pi a})}} \prod_{s=1}^l \sqrt{(s^2 + a^2)} \frac{\Gamma(l+1+\frac{1}{2})}{(2l+1)!} \\ &\times \left[\frac{(2l+1)(l-n)!}{4\pi(l+n)!} \right] j_l\left(-\frac{k\sqrt{2U_p}}{w}\right) P_l^n(0) P_l^n(\cos\theta_k) e^{-m\phi_k} \\ &\times (2\pi)^{\frac{3}{2}} \langle \vec{k} | \phi_i \rangle (E_k + E_B) \end{aligned} \quad (3.277)$$

Using

$$\begin{aligned} \Gamma(l+1+\frac{1}{2}) &= \frac{(2l+1)!}{2^{2l+1} l!} \sqrt{\pi} \\ \prod_{s=1}^l \sqrt{(s^2 + a^2)} &= l! \prod_{s=1}^l \sqrt{1 + \left(\frac{a}{s}\right)^2} \\ P_l^n(0) &= \frac{(-1)^{\frac{l-n}{2}} (l+n)!}{2^l \left(\frac{l-n}{2}\right)! \left(\frac{l+n}{2}\right)!} \end{aligned}$$

We arrive at

$$\begin{aligned} T_{\text{fi}}(n) &= \frac{\sqrt{Z}}{\sqrt{2\pi k}} \sum_{l=n}^* \frac{i^{-l} (-1)^{\frac{l-n}{2}}}{2^l} \sqrt{\frac{8\pi}{a(1-e^{-2\pi a})}} \prod_{s=1}^l \sqrt{1 + \left(\frac{a}{s}\right)^2} \\ &\times \left[\frac{(2l+1)(l-n)!}{4\pi \left(\frac{l+n}{2}\right)! \left(\frac{l-n}{2}\right)!} \right] j_l\left(-\frac{k\sqrt{2U_p}}{w}\right) P_l^n(\cos\theta_k) e^{-m\phi_k} \\ &\times (2\pi)^{\frac{3}{2}} \langle \vec{k} | \phi_i \rangle (E_k + E_B) \end{aligned} \quad (3.278)$$

Finally, the differential momentum distribution of order n , $\frac{d^3W}{d^3k}(n)$, is

$$\frac{d^3W}{d^3k}(n) = 2\pi|T_{\text{fi}}(n)|^2 \quad (3.279)$$

The differential momentum distribution for detection of the emitted electrons in the polarization plane is obtained by setting $\theta_k = \frac{\pi}{2}$ so that

$$\begin{aligned} T_{\text{fi}}(n)|_{\theta_k=\frac{\pi}{2}} &= \frac{\sqrt{Z}}{\sqrt{2\pi}k} \sum_{l=n}^* \frac{i^{-l}(-1)^{l-n}}{2^{2l}} \sqrt{\frac{8\pi}{a(1-e^{-2\pi a})}} \prod_{s=1}^l \sqrt{1 + \left(\frac{a}{s}\right)^2} \\ &\times \left[\frac{(2l+1)(l+n)!(l-n)!}{4\pi[(\frac{l+n}{2})!]^2[(\frac{l-n}{2})!]^2} \right] j_l\left(-\frac{k\sqrt{2U_p}}{w}\right) e^{-in\phi_k} \\ &\times (2\pi)^{\frac{3}{2}} \langle \vec{k} | \phi_i \rangle (E_k + E_B) \end{aligned} \quad (3.280)$$

and therefore

$$\frac{d^3W}{d^3k}(n)|_{\theta_k=\frac{\pi}{2}} = 2\pi|T_{\text{fi}}(n)|_{\theta_k=\frac{\pi}{2}}^2 \quad (3.281)$$

If we denote $\frac{d^3W^{(\text{KFR})}}{d^3k}(n)|_{\theta_k=\frac{\pi}{2}}$ to be the KFR differential momentum distribution for detection of the emitted electrons in the polarization plane, then we have

$$\frac{d^3W^{(\text{KFR})}}{d^3k}(n)|_{\theta_k=\frac{\pi}{2}} = 2\pi|T_{\text{fi}}^{(\text{KFR})}(n)|_{\theta_k=\frac{\pi}{2}}^2 \quad (3.282)$$

where $T_{\text{fi}}^{(\text{KFR})}(n)|_{\theta_k=\frac{\pi}{2}}$ is given by Eq. (2.102)

$$T_{\text{fi}}^{(\text{KFR})}(n)|_{\theta_k=\frac{\pi}{2}} = -\langle \vec{k} | \phi_i \rangle (E_k + E_B) (-1)^n J_n\left(\frac{k\sqrt{2U_p}}{w}\right) e^{-in\phi_k} \quad (3.283)$$

It is quite obvious from the comparison of Eq. (3.280) with Eq. (3.283) that accurate Coulomb effects considerations in the final state wave function leads to upholding angular momentum considerations which in turn significantly alter the momentum distribution of the emitted electrons. We believe that this is the essence of the counterintuitive shifts in the momentum distributions [60,61]. We will plot $\frac{d^3W}{d^3k}|_{\theta_k=\frac{\pi}{2}}$ as given by Eqs. (3.281) and compare it with that of $\frac{d^3W^{(\text{KFR})}}{d^3k}|_{\theta_k=\frac{\pi}{2}}$ as given by Eqs. (2.282) and (3.283). This is will be carried out for future work.

3.4.2 The Case of Linearly Polarized Light

For a linearly polarized light we have

$$\begin{aligned}\vec{A}(t) &= A_0 \hat{e} \cos wt \\ \vec{\alpha}(t) &= \frac{2\sqrt{U_p}}{w} \hat{e} \sin wt = \left(\frac{2\sqrt{U_p}}{w} \sin wt, 0, wt \right) \\ U_1(t) &= \frac{U_p}{2w} \sin 2wt\end{aligned}$$

Therefore

$$\begin{aligned}\Psi_{A,\vec{k}}^{(-)}(\vec{\alpha}) &= \frac{\sqrt{Z}}{\sqrt{2\pi k}} \sum_{l=0}^{\infty} \sum_{m=-l}^l i^l e^{-i\delta_l} \sqrt{\frac{8\pi}{a(1-e^{-2\pi a})}} \prod_{s=1}^l \sqrt{(s^2+a^2)} \frac{(4k \frac{\sqrt{U_p} \sin \varphi}{w})^l}{(2l+1)!} e^{-i2k \frac{\sqrt{U_p} \sin \varphi}{w}} \\ &\times \left[\frac{(2l+1)(l-m)!}{4\pi(l+m)!} \right] {}_1F_1[l+1+ia, 2l+2, 4ik \frac{\sqrt{U_p} \sin \varphi}{w}] P_l^m(1) P_l^m(\cos \theta_k) e^{im\varphi} e^{-im\phi_k}\end{aligned}\quad (3.284)$$

where $\varphi = wt$. The ionization process by linearly polarized light is accompanied with no net transfer of angular momenta and therefore we expect that only the partial wave with magnetic quantum number $m = 0$ contributes to the transition. Thus, Eq. (3.255) for the transition amplitude $T_{fi}(n)$ with the absorption of n photons now becomes

$$\begin{aligned}T_{fi}(n) &= \frac{\sqrt{Z}}{\sqrt{2\pi k}} \sum_{l=0}^{\infty} \sum_{m=-l}^l i^l e^{-i\delta_l} \sqrt{\frac{8\pi}{a(1-e^{-2\pi a})}} \prod_{s=1}^l \sqrt{(s^2+a^2)} \frac{(2\pi)^{\frac{3}{2}} \langle \vec{k} | \phi_i \rangle (E_k + E_B)}{(2l+1)!} \\ &\times \left[\frac{(2l+1)(l-m)!}{4\pi(l+m)!} \right] P_l^m(1) P_l^m(\cos \theta_k) e^{-im\phi_k} \frac{1}{2\pi} \int_0^{2\pi} d\varphi e^{i[\frac{U_p}{2w} \sin 2\varphi - \frac{2\sqrt{U_p}}{w} k \sin \varphi + (n+m)\varphi]} \\ &\times {}_1F_1[l+1+ia, 2l+2, 4l \frac{\sqrt{U_p}}{w} k \sin \varphi] \left(4 \frac{\sqrt{U_p}}{w} k \sin \varphi \right)^l\end{aligned}\quad (3.285)$$

Now since

$$P_l^m(1) = \delta_{m,0}$$

then only the partial wave with the magnetic quantum number $m = 0$ contributes to the transition and therefore we have

$$\begin{aligned}T_{fi}(n) &= \frac{\sqrt{Z}}{\sqrt{2\pi k}} \sum_{l=0}^{\infty} i^l e^{-i\delta_l} \sqrt{\frac{8\pi}{a(1-e^{-2\pi a})}} \prod_{s=1}^l \sqrt{(s^2+a^2)} \frac{(2\pi)^{\frac{3}{2}} \langle \vec{k} | \phi_i \rangle (E_k + E_B)}{(2l+1)!} \\ &\times \left[\frac{(2l+1)}{4\pi} \right] P_l(\cos \theta_k) \frac{1}{2\pi} \int_0^{2\pi} d\varphi e^{i[\frac{U_p}{2w} \sin 2\varphi - \frac{2\sqrt{U_p}}{w} k \sin \varphi + n\varphi]}\end{aligned}$$

$$\times {}_1F_1[l+1+ia, 2l+2, 4i\frac{\sqrt{U_p}}{w}k\sin\varphi] (4\frac{\sqrt{U_p}}{w}k\sin\varphi)^l \quad (3.286)$$

The differential momentum distribution of order n of the emission of an electron of energy $E_k = \frac{k^2}{2}$ in the direction \hat{k} is

$$\frac{d^3W}{d^3k}(n) = 2\pi|T_{\text{fi}}(n)|^2 \quad (3.287)$$

For the case of a linearly polarized laser field, the system has cylindrical symmetry. In cylindrical coordinates we write

$$\frac{d^3W}{d^3k}(n) = \frac{d^3W}{dk_{\perp}dk_{\parallel}d\phi_k k_{\perp}}(n) = 2\pi|T_{\text{fi}}(n)|^2 \quad (3.288)$$

As a result, the two dimensional momentum distribution of order n is

$$\frac{d^2W}{dk_{\perp}dk_{\parallel}}(n) = 4\pi^2|T_{\text{fi}}(n)|^2 k_{\perp} \quad (3.289)$$

where $k_{\perp} = k \sin \theta_k$ and $k_{\parallel} = k \cos \theta_k$ are the perpendicular and parallel components of \vec{k} with respect to the direction of polarization of the laser field. Of course the total two dimensional momentum distribution $\frac{d^2W}{dk_{\perp}dk_{\parallel}}$, is given by

$$\frac{d^2W}{dk_{\perp}dk_{\parallel}} = \sum_{n=n_0}^{\infty} \delta(E_k + E_B + U_p - nw) \frac{d^2W}{dk_{\perp}dk_{\parallel}}(n) \quad (3.290)$$

The differential rate of emitted electrons with momentum parallel to the polarization axis, $\frac{dW}{dk_{\parallel}}$, is

$$\frac{dW}{dk_{\parallel}} = \int_0^{\infty} dk_{\perp} \frac{d^2W}{dk_{\perp}dk_{\parallel}} \quad (3.291)$$

Since

$$\begin{aligned} \delta(f(x)) &= \sum_i \frac{\delta(x-x_i)}{|f'(x_i)|} \\ E_k &= \frac{1}{2}(k_{\perp}^2 + k_{\parallel}^2) = nw - U_p - E_B \end{aligned}$$

where x_i are the zeros of $f(x)$, then, we arrive at

$$\frac{dW}{dk_{\parallel}} = \sum_{n=n_0}^{\infty} 4\pi^2|T_{\text{fi}}(n)|^2 \quad (3.292)$$

If we denote $\frac{d^2W^{(\text{KFR})}}{dk_{\perp}dk_{\parallel}}(n)$ and $\frac{dW^{(\text{KFR})}}{dk_{\parallel}}$ to be the KFR theory analog of Eqs. (3.289) and (3.292) respectively, then we have

$$\frac{d^2W^{(\text{KFR})}}{dk_{\perp}dk_{\parallel}}(n) = 4\pi^2 |T_{\text{fi}}^{(\text{KFR})}(n)|^2 k_{\perp} \quad (3.293)$$

$$\frac{dW^{(\text{KFR})}}{dk_{\parallel}} = \sum_{n=n_0}^{\infty} 4\pi^2 |T_{\text{fi}}^{(\text{KFR})}(n)|^2 \quad (3.294)$$

where $T_{\text{fi}}^{(\text{KFR})}(n)$ as given by Eq. (2.211) to be

$$T_{\text{fi}}^{(\text{KFR})}(n) = -\langle \vec{k} | \phi_i \rangle (E_k + E_B) J_n \left(\frac{2\sqrt{U_p}}{w} k \cos \theta_k, -\frac{U_p}{2w} \right) \quad (3.295)$$

It is quite obvious from the comparison of Eq. (3.286) with Eq. (3.295) that accurate considerations of Coulomb effects in the final state wave function significantly alter the two dimensional momentum distribution as well as the one dimensional momentum distribution along the polarization direction. The experimental findings of Rudenko et al. [74] showed striking features in their two dimensional electron momentum spectra, as well as in the momentum spectra projected onto the direction of the laser polarization. Similar features in the two dimensional electron momentum spectra have been seen in the data of Maharjan et al. [75] for 400–800 nm wavelengths. Moreover precise measurements of ionized electrons by Moshamer et al. [73] showed a clear double peak structure in the electron momentum distribution parallel to the laser polarization for Ne. The numerical calculations of Dimitriou et al. [81] explained that the double peak structure originated from the influence of the Coulomb force on the ionized electron. Furthermore, Chen et al. [76] calculated the the two dimensional electron distributions of multiphoton ionization of atoms by intense laser fields by solving the time dependent Schrödinger equation (TDSE) for different wavelengths and intensities and compared to those predicted by the strong field approximation (SFA). It is shown that the momentum spectra at low energies between the TDSE and SFA are quite different and the differences arise largely from the absence of the long-range Coulomb effects in the SFA. Furthermore, they found that the low energy two dimensional momentum spectra from the TDSE exhibit fanlike features due to a single dominant angular momentum of the low energy electron. The specific dominant angular momentum in turn has been found to be decided by the minimum number of photons needed to ionize

the atom only. We believe that the above conclusions are embedded in our analytical approach. The numerical evaluation of Eq. (3.286) will be carried out for future work and the resulting two dimensional momentum distribution, the one dimensional distribution along the polarization direction and the low energy ionization rates will be compared with those resulting from the strong field approximation; i.e., Eq. (3.295).

3.5 The Simultaneous Angular and Linear Momenta Considerations

We have demonstrated in the previous section that an accurate consideration of Coulomb effects in the final wave function is required to satisfy conservation of angular momentum and to account for the recently observed counterintuitive shifts in the two dimensional linear momentum distributions for both linearly and circularly polarized light [60-61,74-76]. In the ionization process, longitudinal momentum along the direction of propagation is also transferred to the photoelectrons. A quantum mechanical description of the simultaneous transfer of longitudinal and angular momenta to the photoelectrons is required. The motivation for this is the recent observation of the transfer of longitudinal momentum by Smeenck et al. [82]. To achieve this we ought to include Coulomb effects in the final state wave function and to include retardation in the long wavelength approximation.

3.5.1 Longitudinal Momentum Transfer in Multiphoton Ionization by Circularly and Linearly Polarized Laser Fields

We recall the final state wave function, $\Psi_f^{(-)}$, given by Eq. (3.205)

$$\Psi_f^{(-)}(\vec{r}, t) \approx e^{-i \int^t dt' V_L(t')} \Psi_{A,\vec{p}}^{(-)}(\vec{r}, t) \quad (3.296)$$

$$\approx \Psi_{A,\vec{p}}^{(-)}(\vec{r} - \vec{\alpha}(t), t) \quad (3.297)$$

where $\Psi_{A,\vec{p}}^{(-)}(\vec{r}, t)$ is given by

$$\Psi_{A,\vec{p}}^{(-)}(\vec{r}, t) = \frac{e^{\pi a/2} \Gamma(1 + ia)}{(2\pi)^{\frac{3}{2}}} {}_1F_1[-ia, 1, -i(pr + \vec{p} \cdot \vec{r})] e^{i\vec{p} \cdot \vec{r} - iE_p t} \quad (3.298)$$

The transition amplitude from the ground state ϕ_i to final continuum state $\Psi_f^{(-)}$ is

$$(S - 1)_{fi} = -i \int_{-\infty}^{\infty} dt \langle \Psi_f^{(-)} | V_L \phi_i \rangle \quad (3.299)$$

In the long wavelength approximation the expression $e^{i\vec{k}\cdot\vec{r}} = 1 + i\vec{k}\cdot\vec{r} + \dots$ is replaced by unity when the radiation wavelength is large compared to a dimension of length pertinent to the system. Here \vec{k} is the radiation field propagation vector. To consider longitudinal momentum transfer, we need to go beyond just the first term in the series expansion of the exponential. We start by writing

$$\vec{A} = \vec{A}(\varphi); \quad \varphi = \vec{k} \cdot \vec{r} - wt \quad (3.300)$$

Let

$$\vec{\beta}(\varphi) = \int^{\varphi} \vec{A}(\varphi') d\varphi' \quad (3.301)$$

$$\int^{\varphi} \frac{A^2(\varphi')}{2c^2} d\varphi' = U_1(\varphi) + U_p \varphi \quad (3.302)$$

so that

$$\vec{\alpha}(t) = -\frac{\vec{\beta}(\varphi)}{w} \quad (3.303)$$

$$U(t) = \int^t \frac{A^2(\tau)}{2c^2} d\tau = -\frac{1}{w}(U_1(\varphi) + U_p(\varphi)) \quad (3.304)$$

and

$$\Psi_{A,\vec{p}}(\vec{r}) = \frac{1}{(2\pi)^{\frac{3}{2}}} \int d\vec{q} e^{i\vec{q}\cdot\vec{r}} \tilde{\Psi}_{A,\vec{p}}(\vec{q}) \quad (3.305)$$

$$\phi_i(\vec{r}) = \frac{1}{(2\pi)^{\frac{3}{2}}} \int d\vec{q} e^{i\vec{q}\cdot\vec{r}} \tilde{\phi}_i(\vec{q}) \quad (3.306)$$

where $\tilde{\Psi}_{A,\vec{p}}(\vec{q})$ and $\tilde{\phi}_i(\vec{q})$ are the Fourier transforms of $\Psi_{A,\vec{p}}(\vec{r})$ and $\phi_i(\vec{r})$ respectively

$$\tilde{\Psi}_{A,\vec{p}}(\vec{q}) = \frac{1}{(2\pi)^{\frac{3}{2}}} \int d\vec{r} e^{-i\vec{q}\cdot\vec{r}} \Psi_{A,\vec{p}}(\vec{r}) \quad (3.307)$$

$$\tilde{\phi}_i(\vec{q}) = \frac{1}{(2\pi)^{\frac{3}{2}}} \int d\vec{r} e^{-i\vec{q}\cdot\vec{r}} \phi_i(\vec{r}) \quad (3.308)$$

Using the transversality condition

$$\vec{A} \cdot \vec{k} = \frac{\partial \vec{A}}{\partial t} \cdot \vec{k} = \vec{\beta} \cdot \vec{k} = 0 \quad (3.309)$$

we obtain

$$e^{-i \int^t dt' V_L(t')} e^{i \vec{q} \cdot \vec{r}} = e^{-i \int^t dt' V_L(\vec{q}, t')} e^{i \vec{q} \cdot \vec{r}} \quad (3.310)$$

$$V_L e^{i \vec{q} \cdot \vec{r}} = V_L(\vec{q}) e^{i \vec{q} \cdot \vec{r}} \quad (3.311)$$

Then we have

$$\begin{aligned} (S-1)_{\text{fi}} &= \left(-\frac{i}{(2\pi)^3}\right) \int_{-\infty}^{\infty} dt \int d\vec{q} \int d\vec{q}' \int d\vec{r} e^{i(E_p+E_B)t} \tilde{\Psi}_{\mathbf{A},\mathbf{P}}^*(\vec{q}) e^{i \int^t dt' V_L(\vec{q}, t')} \\ &\times \tilde{\phi}_i(\vec{q}') V_L(\vec{q}', t) e^{-i(\vec{q}-\vec{q}') \cdot \vec{r}} \end{aligned} \quad (3.312)$$

Using Eqs. (3.301) and (3.302) yields

$$\begin{aligned} (S-1)_{\text{fi}} &= \left(-\frac{i}{(2\pi)^3}\right) \int_{-\infty}^{\infty} dt \int d\vec{q} \int d\vec{q}' \int d\vec{r} e^{i(E_p+E_B)t} \tilde{\Psi}_{\mathbf{A},\mathbf{P}}^*(\vec{q}) \tilde{\phi}_i(\vec{q}') \\ &\times e^{-i \frac{U_p}{w} (\vec{k} \cdot \vec{r} - wt)} e^{-\frac{i}{w} [\vec{\beta}(\varphi) \cdot \vec{q} + U_1(\varphi)]} V_L(\vec{q}', \varphi) e^{-i(\vec{q}-\vec{q}') \cdot \vec{r}} \end{aligned} \quad (3.313)$$

Now

$$e^{-\frac{i}{w} [\vec{\beta}(\varphi) \cdot \vec{q} + U_1(\varphi)]} V_L(\vec{q}', \varphi)$$

is periodic in φ with a period 2π . Thus we write

$$e^{-\frac{i}{w} [\vec{\beta}(\varphi) \cdot \vec{q} + U_1(\varphi)]} V_L(\vec{q}', \varphi) = \sum_n a_n(\vec{q}, \vec{q}') e^{im\varphi} \quad (3.314)$$

and the Fourier components $a_n(\vec{q}, \vec{q}')$ are

$$a_n(\vec{q}, \vec{q}') = \frac{1}{2\pi} \int_0^{2\pi} e^{-\frac{i}{w} [\vec{\beta}(\varphi) \cdot \vec{q} + U_1(\varphi)] - im\varphi} V_L(\vec{q}', \varphi) d\varphi \quad (3.315)$$

The expression for the transition probability now reads

$$\begin{aligned} (S-1)_{\text{fi}} &= \left(-\frac{i}{(2\pi)^3}\right) \sum_n \int_{-\infty}^{\infty} dt \int d\vec{q} \int d\vec{q}' \int d\vec{r} e^{i(E_p+E_B+U_p-nw)t} \tilde{\Psi}_{\mathbf{A},\mathbf{P}}^*(\vec{q}) \tilde{\phi}_i(\vec{q}') \\ &\times a_n(\vec{q}, \vec{q}') e^{-i[\vec{q}-\vec{q}' - (n - \frac{U_p}{w})\vec{k}] \cdot \vec{r}} \end{aligned} \quad (3.316)$$

The temporal and space integrals yield the energy conserving delta function, $2\pi\delta(E_p + E_B + U_p - nw)$, and the linear momentum conserving delta function, $(2\pi)^3\delta(\vec{q} - \vec{q}' - (n - \frac{U_p}{w})\vec{k})$, respectively. The integral over \vec{q} becomes straightforward and we obtain

$$\begin{aligned} (S-1)_{\text{fi}} &= -2\pi i \sum_n \delta(E_p + E_B + U_p - nw) \int d\vec{q}' a_n(\vec{q}') \\ &\times \tilde{\Psi}_{\mathbf{A},\mathbf{P}}^*(\vec{q}' + (n - \frac{U_p}{w})\vec{k}) \tilde{\phi}_i(\vec{q}') \end{aligned} \quad (3.317)$$

where, using the transversality condition $\vec{\beta} \cdot \vec{k} = 0$,

$$\begin{aligned} a_n(\vec{q}') &= \frac{1}{2\pi} \int_0^{2\pi} d\varphi e^{-\frac{\iota}{w} [\beta(\vec{\varphi}) \cdot \vec{q}' + U_1(\varphi) + U_p \varphi]} \\ &\times e^{-\iota(n - \frac{U_p}{w})\varphi} V_L(\vec{q}', \varphi) \end{aligned} \quad (3.318)$$

Integration by parts gives

$$a_n(\vec{q}') = -(nw - U_p) \frac{1}{2\pi} \int_0^{2\pi} d\varphi e^{-\frac{\iota}{w} [\beta(\vec{\varphi}) \cdot \vec{q}' + U_1(\varphi) + nw\varphi]} \quad (3.319)$$

Substituting Eq. (3.319) into Eq. (3.317) yields

$$\begin{aligned} (S - 1)_{\text{fi}} &= 2\pi\iota \sum_n \delta(E_p + E_B + U_p - nw) (nw - U_p) \frac{1}{2\pi} \int_0^{2\pi} d\varphi e^{-\frac{\iota}{w} [U_1(\varphi) + nw\varphi]} \\ &\times \int d\vec{q}' \tilde{\Psi}_{A, \vec{p}}^*(\vec{q}' + (n - \frac{U_p}{w})\vec{k}) \tilde{\phi}_1(\vec{q}') e^{\iota\vec{\alpha} \cdot \vec{q}'} \end{aligned} \quad (3.320)$$

where we used $\vec{\alpha} = -\vec{\beta}/w$. Now, according to Eq. (3.219), we have previously obtained an expression for $\tilde{\Psi}_{A, \vec{p}}^*(\vec{q}' + (n - \frac{U_p}{w})\vec{k})$

$$\begin{aligned} \tilde{\Psi}_{A, \vec{p}}^*(\vec{q}' + (n - \frac{U_p}{w})\vec{k}) &= \frac{\Gamma(1 - \iota a) e^{\pi a/2}}{2\pi^2} \lim_{\lambda \rightarrow 0} -\frac{\partial}{\partial \lambda} \frac{1}{(\vec{p} - [\vec{q}' + (n - U_p/w)\vec{k}])^2 + \lambda^2} \\ &\times \left[\frac{(\vec{q}' + (n - U_p/w)\vec{k})^2 - (p - \iota\lambda)^2}{(\vec{p} - [\vec{q}' + (n - U_p/w)\vec{k}])^2 + \lambda^2} \right]^{-\iota a} \end{aligned} \quad (3.321)$$

The value of the integral over \vec{q}' in Eq. (3.320) is mainly determined by the poles of the integrand. The poles are $q' = |\vec{p} - (n - U_p/w)\vec{k}| + \iota\lambda$ and $q' = \iota Z$. Moreover, due to the damping of the $e^{\iota\vec{q}' \cdot \vec{\alpha}}$ term in the integral, the contribution due to the pole $q' = |\vec{p} - (n - U_p/w)\vec{k}| + \iota\lambda$ is larger than the pole $q' = \iota Z$. Furthermore, if we carry the process of differentiation with respect to λ we will get a leading term which is identified as a Dirac-delta function, namely

$$\lim_{\lambda \rightarrow 0} \frac{1}{\pi^2} \frac{\lambda}{[(\vec{p} - [\vec{q}' + (n - U_p/w)\vec{k}])^2 + \lambda^2]^2} = \delta(\vec{p} - [\vec{q}' + (n - U_p/w)\vec{k}]) \quad (3.322)$$

Therefore, the value of the above integral is largely due to the pole $\vec{q}' = \vec{p} - (n - U_p/w)\vec{k}$ and $\tilde{\phi}_1(\vec{q}')$ is taken outside the integral and evaluated at $\vec{q}' = \vec{p} - (n - U_p/w)\vec{k}$. Therefore,

Eq. (3.320) now reads

$$\begin{aligned}
(S-1)_{\text{fi}} &= 2\pi i \sum_n \delta(E_p + E_B + U_p - nw) (nw - U_p) \frac{1}{2\pi} \int_0^{2\pi} d\varphi e^{-\frac{i}{w}[U_1(\varphi) + nw\varphi]} \\
&\times \tilde{\phi}_i(\vec{p} - (n - U_p/w)\vec{k}) \int d\vec{q}' \tilde{\Psi}_{A,\vec{p}}^*(\vec{q}' + (n - \frac{U_p}{w})\vec{k}) e^{i\vec{\alpha} \cdot [\vec{q}' + (n - U_p/w)\vec{k}]}
\end{aligned} \tag{3.323}$$

where the transversality condition $\alpha \cdot \vec{k} = 0$ is used. From Eq. (3.305), it is easy to see that the integral over \vec{q}' equals to $(2\pi)^{\frac{3}{2}} \Psi_{A,\vec{p}}^{(-)}(\vec{\alpha})$. Using Eq. (3.298) we obtain

$$\begin{aligned}
(S-1)_{\text{fi}} &= 2\pi i e^{\pi a/2} \Gamma(1 + ia) \sum_n \delta(E_p + E_B + U_p - nw) (nw - U_p) \tilde{\phi}_i(\vec{p} - (n - U_p/w)\vec{k}) \\
&\times \frac{1}{2\pi} \int_0^{2\pi} d\varphi e^{i[\vec{p} \cdot \vec{\alpha}(\varphi) + U_1(\varphi) + n\varphi]} {}_1F_1[-ia, 1, -i(p\alpha(\varphi) + \vec{p} \cdot \vec{\alpha}(\varphi))]
\end{aligned} \tag{3.324}$$

where $\varphi = wt$. The probability amplitude as given by Eq. (3.324) is consistent with the simultaneous conservation of linear and angular momenta.

It is worthwhile to observe that had we set $\tilde{\Psi}_{A,\vec{p}}^*(\vec{q}' + (n - \frac{U_p}{w})\vec{k}) = \delta(\vec{p} - (\vec{q}' + (n - \frac{U_p}{w})\vec{k}))$ then Eq. (3.320) simplifies to

$$\begin{aligned}
(S-1)_{\text{fi}} &= 2\pi i \sum_n \delta(E_p + E_B + U_p - nw) (nw - U_p) \tilde{\phi}_i(\vec{p} - (n - U_p/w)\vec{k}) \\
&\times \frac{1}{2\pi} \int_0^{2\pi} d\varphi e^{i[\vec{p} \cdot \vec{\alpha}(\varphi) + U_1(\varphi) + n\varphi]}
\end{aligned} \tag{3.325}$$

which is in agreement with the expression obtained by Salamin [83].

Now let us shed some light in the physics underneath the mathematical derivation. From the energy-conserving delta function we have

$$E_p = \frac{p^2}{2} = nw - U_p - E_B$$

Also from the momentum-conserving delta function, which results from the space integral, we have

$$\vec{p} = \vec{q} = \vec{q}' + (n - \frac{U_p}{w})\vec{k}$$

where \vec{q}' is the momentum of the initial state. This means that the electron absorbs momentum in the amount $(n - \frac{U_p}{w})\vec{k}$ from the laser field. The absorbed momentum is all in

the longitudinal direction. Assuming \vec{k} along the z axis, then the longitudinal component, p_z ,

$$p_z = (n - \frac{U_p}{w})k \quad (3.326)$$

Since $nw - U_p = E_p + E_B$, and $k = \frac{w}{c}$ then we obtain

$$p_z = \frac{E_p}{c} + \frac{E_B}{c} \quad (3.327)$$

Smeenk et al. [82], on the basis of classical physics, obtained for the net longitudinal momentum after the pulse has passed:

$$p_z = \frac{E_p}{c} \quad (3.328)$$

3.5.2 The Longitudinal Momentum Distribution

Since the experimental data of Smeenk et al. [82] are for circularly polarized laser fields we will outline in detail the calculations for circularly polarized laser fields. In this case, for a circularly polarized light propagating along the z axis we have

$$\frac{1}{2\pi} \int_0^{2\pi} d\varphi e^{i[\vec{p} \cdot \vec{\alpha}(\varphi) + U_1(\varphi) + n\varphi]} = (-1)^n J_n \left(\frac{\sqrt{2U_p}}{w} p \sin \theta_p \right) e^{\pm im\varphi_p} \quad (3.329)$$

where θ_p is the angle that the ejected electron with momentum \vec{p} makes with the z axis, φ_p is the azimuthal angle and the \pm stands for right/left hand polarization respectively. Substituting Eq. (3.329) into Eq. (3.325) yields

$$\begin{aligned} (S - 1)_{\text{fi}} &= 2\pi i \sum_n \delta(E_p + E_B + U_p - nw) (nw - U_p) \tilde{\phi}_i(\vec{p} - (n - U_p/w)\vec{k}) \\ &\times (-1)^n J_n \left(\frac{\sqrt{2U_p}}{w} p \sin \theta_p \right) e^{\pm im\varphi_p} \end{aligned} \quad (3.330)$$

The ionization rate $\bar{\omega}(I)$ at a constant intensity is

$$\begin{aligned} \bar{\omega}(I) &= 2\pi \sum_{n=n_0} \delta(E_p + E_B + U_p - nw) (nw - U_p)^2 |\tilde{\phi}_i(\vec{p} - (n - U_p/w)\vec{k})|^2 \\ &\times |J_n \left(\frac{\sqrt{2U_p}}{w} p \sin \theta_p \right)|^2 \end{aligned} \quad (3.331)$$

where $n_0 = (U_p + E_p)/w$ is the minimum number of photons required for threshold ionization and the final momentum $p = \sqrt{2E_p} = (nw - U_p - E_p)$.

In an actual experiment the intensity of the laser pulse varies within an envelope. For a Gaussian pulse, as the case of the experiment of Smeenk et al. [82], the intensity $I(\rho, z)$ distribution within the focal volume is [84]

$$I(\rho, z) = I_0 \left(\frac{\omega_0}{\omega(z)} \right)^2 e^{-\frac{2\rho^2}{\omega(z)^2}} \quad (3.332)$$

where

$$\omega(z) = \omega_0 [1 + (z/z_0)^2]^{\frac{1}{2}} \quad (3.333)$$

and $\omega_0 = \sqrt{\lambda z_0/\pi}$ is the Rayleigh range. The focal volume consists of surfaces of constant intensity. The differential volume element is a shell between two surfaces of constant intensity I and $I + dI$. Atoms lying within a given differential volume element are ionized at a constant intensity I .

In terms of the longitudinal p_z and transverse p_\perp components, the quantum mechanical ionization rate at a constant intensity is

$$\tilde{\omega}(I) = 2\pi |\phi(\vec{p} - (nw - U_p)(k/w)\hat{e}_z)|^2 \sum_{n=n_0}^{\infty} \delta\left(\frac{p_\perp^2}{2} + \frac{p_z^2}{2} + E_B + U_p - nw\right) (nw - U_p)^2 J_n^2\left(\frac{\sqrt{2U_p} p_\perp}{w}\right) \quad (3.334)$$

The Fourier transform of the ground state wave function $|\phi(\vec{p})|$ is

$$\phi(\vec{p} - (nw - U_p)(k/w)\hat{e}_z) = \frac{\sqrt{8Z^5}}{\pi} \frac{1}{[Z^2 + p_z^2 + p_\perp^2 + (nw - U_p)^2(k/w)^2 - 2(nw - U_p)(k/w)p_z]^2} \quad (3.335)$$

where Z is the ionic charge. The total ionization rate $W(I)$ at a constant intensity I is

$$W(I) = \int d\vec{p} \tilde{\omega}(I) = \int d\varphi dp_z dp_\perp p_\perp \tilde{\omega}(I) \quad (3.336)$$

where $d\vec{p} = d\varphi dp_z dp_\perp p_\perp$ is the volume element in cylindrical coordinates. The total ionization rate $\frac{dW(I)}{dp_z}$ per unit of longitudinal momentum at a constant intensity I is

$$\frac{dW(I)}{dp_z} = 2\pi \int_0^\infty dp_\perp p_\perp \tilde{\omega}(I) \quad (3.337)$$

Due to the presence of the Dirac-delta function, the integral over dp_\perp is evaluated to yield

$$\frac{dW(I)}{dp_z} = 32 Z^5 \sum_{n=n_0}^{\infty} \frac{(nw - U_p)^2 J_n^2[\sqrt{4U_p(nw - U_p - E_B - \frac{p_z^2}{2})}/w]}{[Z^2 + 2(nw - U_p - E_B) + (nw - U_p)/c^2 - 2(nw - U_p)p_z/c]^4} \quad (3.338)$$

If ρ_d denotes the density of the atoms within the focal volume then, within the focal volume the total number of electrons generated per unit time per unit of longitudinal momentum is

$$\frac{d^2N}{dt dp_z} = \rho_d \int dV \frac{dW(I)}{dp_z} = \rho_d \int_0^{I_0} \frac{dV}{dI} \frac{dW(I)}{dp_z} dI \quad (3.339)$$

where it is assumed that the density of atoms is kept constant. The space integration over the focal volume is replaced by integration over the intensity spectrum within the focal volume corresponding to the sum of all contributions from all differential volume shells of constant intensity I . Now since

$$\frac{dV}{dI} = -\frac{\pi\omega_0^2 z_0}{3} I^{-\frac{5}{2}} \sqrt{I_0 - I} (2I + I_0) \quad (3.340)$$

then

$$\frac{d^2N}{dt dp_z} = \frac{\pi\omega_0^2 z_0 \rho_d}{3} \int_0^{I_0} \frac{dI}{I^{\frac{5}{2}}} \sqrt{I_0 - I} (2I + I_0) \frac{dW(I)}{dp_z} \quad (3.341)$$

The total number of electrons generated per unit of longitudinal momentum is then

$$\frac{dN}{dp_z} = \int_{-\infty}^{\infty} dt \frac{d^2N}{dt dp_z} \quad (3.342)$$

For a Gaussian pulse with temporal width τ the intensity profile is [84]

$$I(\rho, z, t) = I(\rho, z) e^{-\frac{(z-ct)^2}{c^2\tau^2}} \quad (3.343)$$

and therefore we obtain

$$\frac{dN}{dp_z} = 2\pi\tau\rho_d z_0 \omega_0^2 \int_0^{I_0} \frac{dI}{I^{\frac{5}{2}}} \sqrt{I_0 - I} \frac{dW(I)}{dp_z} \int_0^1 d\eta [I + (I_0 - I)\eta^2] \left[\ln \frac{I_0}{I + (I_0 - I)\eta^2} \right]^{\frac{1}{2}} \quad (3.344)$$

For a short pulse in the femtosecond range with a distribution profile [82]

$$I = I_0 e^{-\frac{4\ln 2}{c^2\tau^2}(z-ct)^2} \quad (3.345)$$

and, for such a profile, if we assume an average intensity \bar{I} at ionization which is given by

$$\bar{I} \approx \frac{1}{\tau} \int_0^{\infty} I_0 e^{-\frac{4\ln 2}{c^2\tau^2}(z-ct)^2} dt = \frac{\sqrt{\pi}}{4\sqrt{\ln 2}} I_0 \quad (3.346)$$

then the integral over I in Eq. (3.344) can be disposed of by putting $I = \bar{I}$. This gives

$$\frac{dN}{dp_z}(\bar{I}) = 2\pi\tau\rho_d z_0 \omega_0^2 \frac{I_0}{\bar{I}^{\frac{5}{2}}} \sqrt{I_0 - \bar{I}} \frac{dW(\bar{I})}{dp_z} \int_0^1 d\eta [\bar{I} + (I_0 - \bar{I})\eta^2] \left[\ln \frac{I_0}{\bar{I} + (I_0 - \bar{I})\eta^2} \right]^{\frac{1}{2}} \quad (3.347)$$

where $I_0 = 4\sqrt{\frac{\ln 2}{\pi}}\bar{I}$. Now, if we define

$$G(\bar{I}) = \int_0^1 d\eta [\bar{I} + (I_0 - \bar{I})\eta^2] \left[\ln \frac{I_0}{\bar{I} + (I_0 - \bar{I})\eta^2} \right]^{\frac{1}{2}} \quad (3.348)$$

we obtain

$$\frac{dN}{dp_z}(\bar{I}) = 2\pi\tau\rho_d z_0 \omega_0^2 \frac{I_0}{\bar{I}^{\frac{5}{2}}} \sqrt{I_0 - \bar{I}} \frac{dW(\bar{I})}{dp_z} G(\bar{I}) \quad (3.349)$$

Substituting Eq. (3.338), for $\frac{dW(\bar{I})}{dp_z}$, into Eq. (3.347) we finally obtain

$$\begin{aligned} \frac{dN}{dp_z}(\bar{I}) &= 32 Z^5 2\pi\tau\rho_d z_0 \omega_0^2 \frac{I_0}{\bar{I}^{\frac{5}{2}}} \sqrt{I_0 - \bar{I}} G(\bar{I}) \\ &\times \sum_{n=n_0}^{\infty} \frac{(nw - \bar{U}_p)^2 J_n^2[\sqrt{4\bar{U}_p(nw - \bar{U}_p - E_B - \frac{p_z^2}{2})}/w]}{[Z^2 + 2(nw - \bar{U}_p - E_B) + (nw - \bar{U}_p)/c^2 - 2(nw - \bar{U}_p)p_z/c]^4} \end{aligned} \quad (3.350)$$

where \bar{U}_p signifies the value of the ponderomotive energy at the average intensity \bar{I} at ionization.

The sum in Eq. (3.350) can be terminated at a cutoff value n_{cut} , where convergence is reached. In the case of ionization by circularly polarized light at constant intensity, the photoelectron energy spectrum peaks at energy $E_p = U_p$. Since $n_0 = (U_p + E_B)/w$, corresponding to threshold ionization, then the cutoff value can be safely taken to be $n_{\text{cut}} = 3(2U_p + E_B)/w$. Thus

$$\begin{aligned} \frac{dN}{dp_z}(\bar{I}) &= 32 Z^5 2\pi\tau\rho_d z_0 \omega_0^2 \frac{I_0}{\bar{I}^{\frac{5}{2}}} \sqrt{I_0 - \bar{I}} G(\bar{I}) \\ &\times \sum_{n=n_0}^{n_{\text{cut}}} \frac{(nw - \bar{U}_p)^2 J_n^2[\sqrt{4\bar{U}_p(nw - \bar{U}_p - E_B - \frac{p_z^2}{2})}/w]}{[Z^2 + 2(nw - \bar{U}_p - E_B) + (nw - \bar{U}_p)/c^2 - 2(nw - \bar{U}_p)p_z/c]^4} \end{aligned} \quad (3.351)$$

where

$$n_0 = \frac{\bar{U}_p + E_B}{w}, \quad n_{\text{cut}} = 3\frac{(2\bar{U}_p + E_B)}{w}, \quad I_0 = 4\sqrt{\frac{\ln 2}{\pi}}\bar{I}$$

and $G(\bar{I})$ is given by Eq. (3.348).

We will discuss briefly the linear polarization case. Here, the ionization rate at a

constant intensity is

$$\begin{aligned} \tilde{\omega}(I) &= \sum_{n=n_0}^{\infty} \delta\left(\frac{p_{\perp}^2}{2} + \frac{p_z^2}{2} + E_B + U_p - nw\right) (nw - U_p)^2 2\pi |\phi(\vec{p} - (nw - U_p)(k/w)\hat{e}_z)|^2 \\ &\times \tilde{J}_n^2\left(\frac{2\sqrt{U_p}p_{\perp}}{w}, -\frac{U_p}{2w}\right) \end{aligned} \quad (3.352)$$

where \tilde{J}_n is a generalized Bessel function. Carrying out the same mathematical approach as that of the circular polarization case we obtain

$$\begin{aligned} \frac{dN}{dp_z}(\bar{I}) &= 32 Z^5 2\pi\tau\rho_d z_0 \omega_0^2 \frac{I_0}{\bar{I}^{\frac{5}{2}}} \sqrt{I_0 - \bar{I}} G(\bar{I}) \\ &\times \sum_{n=n_0}^{n_{\text{cut}}} \frac{(nw - \bar{U}_p)^2 \tilde{J}_n^2[2\sqrt{2\bar{U}_p}(nw - \bar{U}_p - E_B - \frac{p_z^2}{2})/w, -\frac{\bar{U}_p}{2w}]}{[Z^2 + 2(nw - \bar{U}_p - E_B) + (nw - \bar{U}_p)/c^2 - 2(nw - \bar{U}_p)p_z/c]^4} \end{aligned} \quad (3.353)$$

where the cutoff value is safely taken to be $n_{\text{cut}} = 3(3\bar{U}_p + E_B)/w$ due to the fact the photoelectron energy spectrum extends from 0 to $2U_p$ (the low energy plateau).

Now, we can see qualitatively that the longitudinal distributions given by Eqs. (3.351) (circular polarization case) and (3.353) (linear polarization case) produces net longitudinal momentum. This is because Eqs. (3.351) and (3.353) are not symmetric around $p_z = 0$ and therefore the center of the distributions will have a net $p_z > 0$. Furthermore, the distribution in the circularly polarized case is determined by the square of Bessel function, so that the center is shifted away from $p_z = 0$ (similar to the energy spectrum which is shifted away from $E_p = 0$ and peaks around $E_p = U_p$). In the linear polarization case, the distribution is determined by the square of the generalized Bessel function, in which case the distribution is shifted away but not as far as the circular case (in the linear case the energy spectrum is concentrated in the vicinity of $E_p \approx 0$ and extends up to $2U_p$). This is qualitatively in agreement with the experimental findings of Smeenk et al. [82] (see Figs. 3.4 and 3.5).

In future work, the numerical evaluation of Eqs. (3.351) and (3.353) will be carried out.

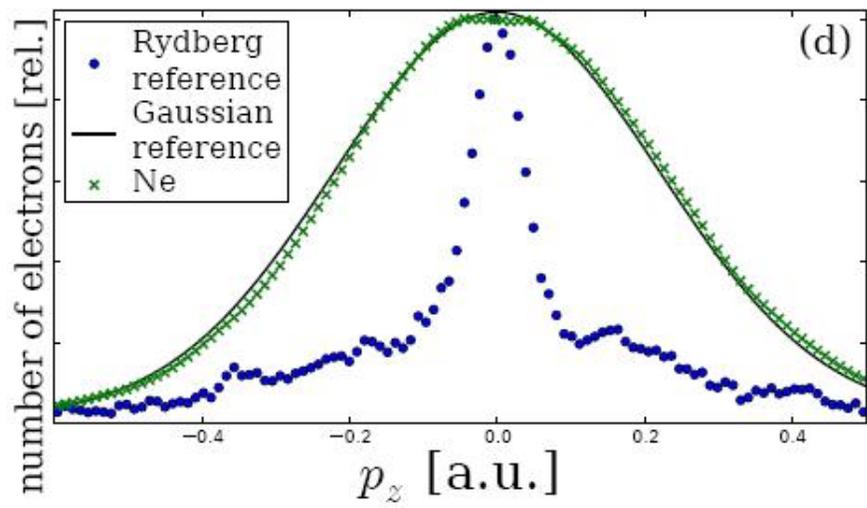


Figure 3.4: The measured Ne photoelectron distribution (crosses) is compared to the Rydberg reference distribution (dots) and a reference Gaussian distribution centered at $p_z = 0$. The centre of the Ne distribution has a net $p_z > 0$. Courtesy of Smeenk et al. [82].

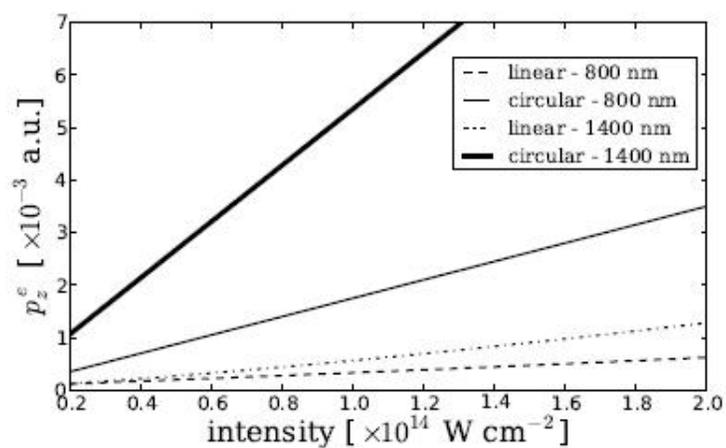


Figure 3.5: Net photoelectron longitudinal momentum p_z vs laser intensity calculated for linear and circularly polarized light. Courtesy of Smeenk et al. [82].

3.5.3 The ponderomotive Scattering Angle

As a consequence of including retardation corrections to the long wavelength approximation, we arrived at Eqs. (3.325) and (3.326) for the acquired longitudinal momentum, p_z ,

$$p_z = \left(n - \frac{U_p}{w}\right)k \quad (3.354)$$

and

$$p_z = \frac{E_p}{c} + \frac{E_B}{c} \quad (3.355)$$

respectively. These equations imply that following ionization a photoelectron which is expected to move in the direction of the polarization vector of the field is scattered away from that direction due to acquired longitudinal momentum. This is what is called ponderomotive scattering. Thus the ponderomotive scattering angle θ_d is given by

$$\cos \theta_d = \frac{p_z}{p} = \sqrt{\frac{E_p}{2c^2}} + \frac{E_B}{\sqrt{2c^2 E_p}} \quad (3.356)$$

It is the objective of this discussion to determine the ponderomotive scattering angle, θ_d . We recall Eq. (3.331) for the ionization rate at constant intensity by circularly polarized light

$$\begin{aligned} \bar{\omega}(I) &= 2\pi \sum_{n=n_0} \delta(E_p + E_B + U_p - nw) (nw - U_p)^2 |\tilde{\phi}_i(\vec{p} - (n - U_p/w)\vec{k})|^2 \\ &\times |J_n(\frac{\sqrt{2U_p}}{w} p \sin \theta_p)|^2 \end{aligned} \quad (3.357)$$

The total ionization rate \bar{W} is thus

$$\bar{W} = \int d\vec{p} \bar{\omega}$$

Thus the ionization rate $\frac{d\bar{W}}{dE_p}$ per unit energy to detect an electron in the polarization plane is

$$\frac{d\bar{W}}{dE_p} = 2\pi \sqrt{2E_p} \bar{\omega}(I)|_{\theta_p=\pi/2} \quad (3.358)$$

Assuming a Gaussian intensity profile, then within the focal volume the total number of electrons generated per unit time per unit of energy in the polarization plane is

$$\frac{d^2 N}{dt dE_p} = \rho_d \int dV \frac{d\bar{W}(I)}{dE_p} = \rho_d \int_0^{I_0} \frac{dV}{dI} \frac{d\bar{W}(I)}{dE_p} dI \quad (3.359)$$

and the number of electrons generated per unit of energy in the polarization plane

$$\frac{dN}{dE_p} = \int_{-\infty}^{\infty} dt \frac{d^2N}{dt dE_p} \quad (3.360)$$

Proceeding in a similar fashion as we did earlier in the discussion of longitudinal distribution, we arrive at

$$\frac{dN}{dE_p}(\bar{I}) = 2\pi\tau\rho_d z_0 \omega_0^2 \frac{I_0}{\bar{I}^{\frac{5}{2}}} \sqrt{I_0 - \bar{I}} \frac{d\bar{W}(\bar{I})}{dE_p} G(\bar{I}) \quad (3.361)$$

If N_t denotes the total number of electrons with energy $E_p \geq 0$ in the polarization plane

$$N_t = \int_0^{\infty} dE_p \frac{dN}{dE_p}(\bar{I}) \quad (3.362)$$

Then the average kinetic energy of electrons in the polarization plane is

$$\begin{aligned} \bar{E}_p &= \frac{1}{N_t} \int_0^{\infty} dE_p E_p \frac{dN}{dE_p}(\bar{I}) \\ &= \frac{\int_0^{\infty} dE_p E_p \frac{d\bar{W}(\bar{I})}{dE_p}}{\int_0^{\infty} dE_p \frac{d\bar{W}(\bar{I})}{dE_p}} \end{aligned} \quad (3.363)$$

Now since

$$\tilde{\phi}_i(\vec{p} - (n - U_p/w)\vec{k}) = \frac{\sqrt{8Z^5}}{\pi} \frac{1}{[Z^2 + (\vec{p} - (n - U_p/w)\vec{k})^2]^2} \quad (3.364)$$

then using Eqs. (3.357) and (3.358) we have

$$\frac{d\bar{W}(\bar{I})}{dE_p} = 32Z^5 \sum_{n=n_0}^{\infty} \delta(E_p + E_B + \bar{U}_p - nw) \sqrt{2E_p} \frac{(nw - \bar{U}_p)^2 J_n^2(\frac{2}{w}\sqrt{\bar{U}_p E_p})}{[Z^2 + 2E_p + (nw - \bar{U}_p)^2/c^2]^2} \quad (3.365)$$

Therefore

$$\int_0^{\infty} dE_p E_p \frac{d\bar{W}(\bar{I})}{dE_p} = 32Z^5 \sum_{n=n_0}^{\infty} \sqrt{2}(E_p)^{\frac{3}{2}} \frac{(nw - \bar{U}_p)^2 J_n^2(\frac{2}{w}\sqrt{\bar{U}_p E_p})}{[Z^2 + 2E_p + (nw - \bar{U}_p)^2/c^2]^2} \quad (3.366)$$

and

$$\int_0^{\infty} dE_p \frac{d\bar{W}(\bar{I})}{dE_p} = 32Z^5 \sum_{n=n_0}^{\infty} \sqrt{2E_p} \frac{(nw - \bar{U}_p)^2 J_n^2(\frac{2}{w}\sqrt{\bar{U}_p E_p})}{[Z^2 + 2E_p + (nw - \bar{U}_p)^2/c^2]^2} \quad (3.367)$$

so that

$$\bar{E}_p = \frac{\sum_{n=n_0}^{\infty} \sqrt{2}(E_p)^{\frac{3}{2}} \frac{(nw - \bar{U}_p)^2 J_n^2(\frac{2}{w}\sqrt{\bar{U}_p E_p})}{[Z^2 + 2E_p + (nw - \bar{U}_p)^2/c^2]^2}}{\sum_{n=n_0}^{\infty} \sqrt{2E_p} \frac{(nw - \bar{U}_p)^2 J_n^2(\frac{2}{w}\sqrt{\bar{U}_p E_p})}{[Z^2 + 2E_p + (nw - \bar{U}_p)^2/c^2]^2}} \quad (3.368)$$

where $E_p = nw - \bar{U}_p - E_B$ and \bar{U}_p is the ponderomotive energy at the average intensity at ionization. Using Eq. (3.355) and (3.356), then the net longitudinal momentum after the pulse and the ponderomotive scattering angle θ_d are:

$$p_z = \frac{\bar{E}_p}{c} + \frac{E_B}{c} \quad (3.369)$$

and

$$\cos \theta_d = \frac{p_z}{p} = \sqrt{\frac{\bar{E}_p}{2c^2}} + \frac{E_B}{\sqrt{2c^2 \bar{E}_p}} \quad (3.370)$$

respectively and where \bar{E}_p is given by Eq. (3.368).

Now for the linear polarization case, the ionization rate at a constant intensity $\bar{\omega}(I)$ is

$$\begin{aligned} \bar{\omega}(I) &= 2\pi \sum_{n=n_0} \delta(E_p + E_B + U_p - nw) (nw - U_p)^2 |\tilde{\phi}_1(\vec{p} - (n - U_p/w)\vec{k})|^2 \\ &\times |\tilde{J}_n[\frac{2\sqrt{U_p}}{w} p \cos \theta_p, -\frac{U_p}{2w}]|^2 \end{aligned} \quad (3.371)$$

where \tilde{J}_n is a generalized Bessel function and θ_p is the angle the free electron with momentum \vec{p} makes with the polarization direction. Carrying out the same mathematical manipulations, similar to what we did for the circular polarization case, then the average kinetic energy of electrons \bar{E}_p along the polarization axis is

$$\bar{E}_p = \frac{\sum_{n=n_0}^{\infty} \sqrt{2}(E_p)^{\frac{3}{2}} \frac{(nw - \bar{U}_p)^2 \tilde{J}_n^2[\frac{2}{w} \sqrt{2\bar{U}_p} E_p, -\frac{\bar{U}_p}{2w}]}{[Z^2 + 2E_p + (nw - \bar{U}_p)^2/c^2]^2}}{\sum_{n=n_0}^{\infty} \sqrt{2E_p} \frac{(nw - \bar{U}_p)^2 \tilde{J}_n^2[\frac{2}{w} \sqrt{2\bar{U}_p} E_p, -\frac{\bar{U}_p}{2w}]}{[Z^2 + 2E_p + (nw - \bar{U}_p)^2/c^2]^2}} \quad (3.372)$$

Similar to their respective photoelectron spectra, \bar{E}_p is determined by the square of Bessel function for circularly polarized laser fields and the square of generalized Bessel function for linearly polarized fields. This means that \bar{E}_p is larger for the case of circular polarization than that of linear polarization. Therefore in accordance with Eq. (3.369) a circularly polarized laser fields deliver a larger net longitudinal momentum than a linearly polarized one, which is qualitatively in agreement with the findings of Smeenck et al. [82].

The numerical evaluation of Eqs. (3.368) and (3.372) will be carried out for future work.

3.6 High Harmonic Generation (HHG)

Similar to our treatment of ATI, we will utilize the fast Fourier transform method and the recently introduced method [67,68] for the accurate numerical evaluation of slowly decaying highly oscillatory functions that extend throughout the half-plane. This will enable an accurate numerical determination of the quantum mechanical cutoff law for HHG.

We consider an atom with a single active electron under the influence of a linearly polarized laser field. In the velocity gauge, we recall the Schrödinger equation (3.1)

$$\left(i\frac{\partial}{\partial t} - H_0 - V_A - V_L\right)\Psi = 0 \quad (3.373)$$

Similar to Lowenstein et al. [30], we assume laser parameters such that the following conditions are valid:

- (1) The contribution to the evolution of the system of all bound states except the ground state ϕ_i can be neglected.
- (2) The depletion of the ground state can be neglected.
- (3) In the continuum, the dynamics of the electron is dominated by the laser field with no effect of V_A .

Based on the above assumptions we write

$$|\Psi\rangle = |\phi_i\rangle + \int d\vec{q} B(\vec{q}, t) |\Psi_{A,\vec{q}}\rangle \quad (3.374)$$

where, as a consequence of condition (2), we set the amplitude of the ground state to ≈ 1 and $B(\vec{q}, t)$ are the amplitudes of the continuum states $|\Psi_{A,\vec{q}}\rangle$. These continuum states satisfy

$$\left(\frac{q^2}{2} - H_0 - V_A\right) |\Psi_{A,\vec{q}}\rangle = 0 \quad (3.375)$$

Substituting Eq. (3.374) into Eq. (3.373) we obtain

$$\int d\vec{q} \left(i\frac{\partial B(\vec{q}, t)}{\partial t} - \langle \Psi_{A,\vec{q}} | V_L | \phi_i \rangle - \frac{q^2}{2} B(\vec{q}, t) - B(\vec{q}, t) V_L \right) |\Psi_{A,\vec{q}}\rangle = 0 \quad (3.376)$$

Utilizing the strong field approximation (condition (3)), we replace $|\Psi_{A,\vec{q}}\rangle$ with a plane wave $|\vec{q}\rangle$ so that

$$V_L |\Psi_{A,\vec{q}}\rangle \approx V_L |\vec{q}\rangle = V_L(\vec{q}) |\vec{q}\rangle \quad (3.377)$$

Therefore the amplitudes $B(\vec{q}, t)$ now satisfy

$$\frac{\partial B(\vec{q}, t)}{\partial t} + \imath \left[\frac{q^2}{2} + V_L(\vec{q}) \right] B(\vec{q}, t) = -\imath V_L(\vec{q}) \langle \vec{q} | \phi_i \rangle e^{\imath E_B t} \quad (3.378)$$

or

$$\frac{\partial}{\partial t} \left[B(\vec{q}, t) e^{\imath \int_{-\infty}^t d\tau \left[\frac{q^2}{2} + V_L(\vec{q}) \right]} \right] = -\imath e^{\imath \int_{-\infty}^t d\tau \left[\frac{q^2}{2} + V_L(\vec{q}) \right]} V_L(\vec{q}) \langle \vec{q} | \phi_i \rangle e^{\imath E_B t} \quad (3.379)$$

Integration by parts gives

$$B(\vec{q}, t) = -\imath \langle \vec{q} | \phi_i \rangle \int_{-\infty}^t dt' V_L(\vec{q}, t') e^{\imath E_B t'} e^{-\imath S(\vec{q}, t, t')} \quad (3.380)$$

where

$$S(\vec{q}, t, t') = \frac{1}{2} \int_{t'}^t d\tau \left[\vec{q} + \frac{1}{c} \vec{A}(\tau) \right]^2 \quad (3.381)$$

is the semiclassical action for the propagation of the electron from t' to t .

For a linearly polarized laser field along the x axis we have

$$\vec{A}(t) = A_0 \hat{x} \cos \omega t$$

The x component of the time dependent dipole moment is

$$X(t) = \langle \Psi | x | \Psi \rangle \quad (3.382)$$

As we have shown in the discussion of ATI, continuum-continuum transitions play a significant role. The off-shell continuum-continuum transitions contribute to the high energy plateau, whereas the on-shell transitions affect the low energy electrons. In the case of HHG they are unimportant and we will neglect them. Allowing only transitions back to the ground state we have

$$X(t) = \int d\vec{q} B(\vec{q}, t) \langle \vec{q} | x | \phi_i \rangle + \text{c.c} \quad (3.383)$$

where C.C means complex conjugate. Substituting Eq. (3.380) into Eq. (3.383) we obtain

$$X(t) = -\imath \int_{-\infty}^t dt' \int d\vec{q} \langle \vec{q} | \phi_i \rangle V_L(\vec{q}, t') e^{\imath E_B t'} e^{-\imath S(\vec{q}, t, t')} \langle \vec{q} | x | \phi_i \rangle + \text{c.c} \quad (3.384)$$

Setting $\tau = t - t'$ then Eq. (3.384) now reads

$$X(t) = \imath \int_0^\infty d\tau \int d\vec{q} \langle \vec{q} | \phi_i \rangle V_L(\vec{q}, t - \tau) e^{\imath E_B (t - \tau)} e^{-\imath S(\vec{q}, t, \tau)} \langle \vec{q} | x | \phi_i \rangle + \text{c.c} \quad (3.385)$$

where now $S(\vec{q}, t, \tau)$ is the semiclassical action for the propagation of an electron from the $t - \tau$ to t and is given by

$$S(\vec{q}, t, \tau) = \frac{1}{2} \int_{t-\tau}^t dt' [\vec{q} + \frac{1}{c} \vec{A}(t')]^2 \quad (3.386)$$

The harmonic strength X_{2K+1} is determined by

$$X_{2K+1} = \frac{1}{2\pi} \int_0^{2\pi} d\varphi X(\varphi) e^{i(2K+1)\varphi} \quad (3.387)$$

where $\varphi = wt$. Substituting Eq. (3.385) into Eq. (3.387) we obtain

$$\begin{aligned} X_{2K+1} &= \frac{1}{2\pi} \int_0^{2\pi} d\varphi e^{i(2K+1+\frac{E_B}{w})\varphi} \iota \int_0^\infty d\tau \int d\vec{q} \langle \vec{q} | \phi_i \rangle V_L(\vec{q}, \varphi - \tau) e^{-iE_B \tau} \\ &\times e^{-iS(\vec{q}, \varphi, \tau)} \langle \vec{q} | x | \phi_i \rangle + \text{C.C} \end{aligned} \quad (3.388)$$

Similar to our treatment of ATI, the integral over \vec{q} is carried out analytically by the saddle-point method yielding

$$\begin{aligned} X_{2K+1} &= \frac{1}{2\pi} \int_0^{2\pi} d\varphi e^{i(2K+1+\frac{E_B}{w})\varphi} \iota \int_0^\infty d\tau \left(\frac{2\pi}{i\tau + \epsilon} \right)^{\frac{3}{2}} \langle \vec{q}_s | \phi_i \rangle V_L(\vec{q}_s, \varphi - \tau) \\ &\times e^{-iE_B \tau} e^{-iS(\vec{q}_s, \varphi, \tau)} \langle \vec{q}_s | x | \phi_i \rangle + \text{c.c} \end{aligned} \quad (3.389)$$

where, \vec{q}_s is the solution of $\vec{\nabla}_{\vec{q}} S(\vec{q}, \varphi, \tau) = 0$

$$\vec{q}_s = \frac{1}{\tau} [\vec{\alpha}(\varphi - \tau) - \alpha(\varphi)] \quad (3.390)$$

Equation (3.389) is mathematically similar to equation (3.183) of ATI. To derive the exact quantum cutoff law in the limit $U_p \rightarrow \infty$, Lewenstein et al. [30] evaluated the remaining integrals over τ and φ analytically using the saddle point approximation. Since Eq. (3.389) is mathematically similar Eq. (3.183) of ATI, then we will utilize the recently introduced method [67,68] for the accurate numerical evaluation of slowly decaying highly oscillatory functions that extend throughout the half-plane. The integral over τ will be evaluated using this method, and then the fast Fourier transform method will be used to evaluate the integral over φ . This will enable an accurate numerical determination of the quantum mechanical cutoff law for HHG. However, this will be carried out for future work.

Chapter 4

Numerical Results and Discussion

From the *ab initio* formulation, which we presented in detail in chapter 3, we concluded that the high energy plateau of the photoelectron spectra is due to rescattering by a short range potential, and the long-range Coulomb potential affects the low energy electrons. Based on this conclusion, we developed an *ad hoc* formulation of ATI, in which we assumed that the influence of the electromagnetic field is to split the atomic potential into two parts: a short range V_s , which is responsible for the high energy plateau, and a long-range Coulomb potential V_c , which affects the low energy electrons. Here, we will present the results of the numerical calculations for the differential ionization rate as a function of the outgoing electron kinetic energy in units of U_p , for the laser parameters used in the experiment by Walker et al. [13]. These parameters are: the intensity, $I = 10^{15}\text{W/cm}^2$, and the photon energy, $w = 1.58\text{eV}$. We will present the results for a monochromatic linearly polarized laser field, for a hydrogen atom in the ground state, and for $V_s = -e^{-r}/r$. Since the laser parameters used in the experiment by Walker et al. [13] are suitable for the tunneling domain, our results include no Coulomb effects. The differential ionization rate of order n as a function of energy is

$$\omega_{\text{fi}}(n, \theta_{\mathbf{k}}) = 2\pi k(n) |T_{\text{fi}}(n)|^2 \quad (4.1)$$

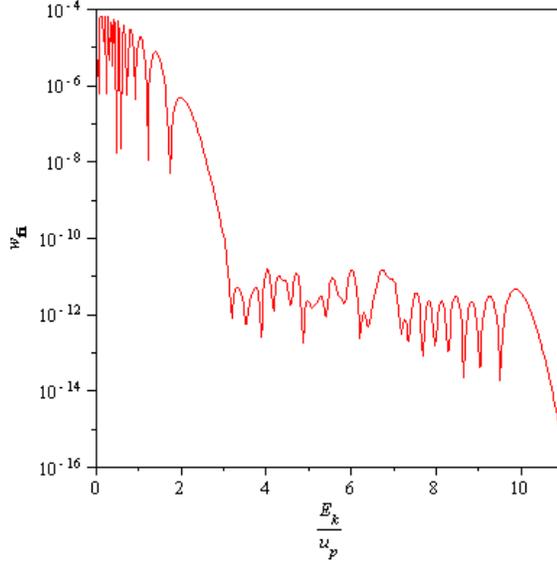


Figure 4.1: Differential ionization rates w_{fi} , in atomic units, of the hydrogen atom as a function of the kinetic energy of electron in units of U_p for $\theta_k = 0^\circ$. The cutoff at $10U_p$.

where, $T_{fi}(n)$ is given by Eq. (3.183).

In Fig. 4.1 we present the differential ionization rate corresponding to the angle $\theta_k = 0^\circ$ between the polarization axis of the laser field and the momentum of the ionized electron. Fig. 4.1 clearly shows a first plateau, corresponding to the low energy electrons, which extend up to $2U_p$, and a second high energy plateau which has a sharp cutoff at $10U_p$. The cutoff position depends on the angle of emission θ_k .

In Fig. 4.2 the ionization rate corresponds to $\theta_k = 10^\circ$. Similar to Fig 4.1, the first plateau extend up to $2U_p$; however the second plateau has a cutoff at $9.6U_p$, which is lower than the cutoff at $10U_p$ for $\theta_k = 0^\circ$.

In Figs. 4.3, 4.4, and 4.5 the ionization rates at the emission angles $\theta_k = 20^\circ, 30^\circ$, and 40° are presented. One can see that the cutoff energy decreases with increasing θ_k . They are at $9U_p$, $8U_p$, and $6.6U_p$ for $\theta_k = 20^\circ, 30^\circ$, and 40° respectively. The results presented in Figs. 4.1–4.5 are in agreement with the findings of Walker et al. [13] (see Figs. 4.7 and 4.8), and the theoretical results of Milošević et al. [59] (see Fig. 4.9).

In Fig. 4.6 the ionization rates at the emission angles $\theta_k = 0^\circ, 10^\circ, 20^\circ, 30^\circ$, and 40° are

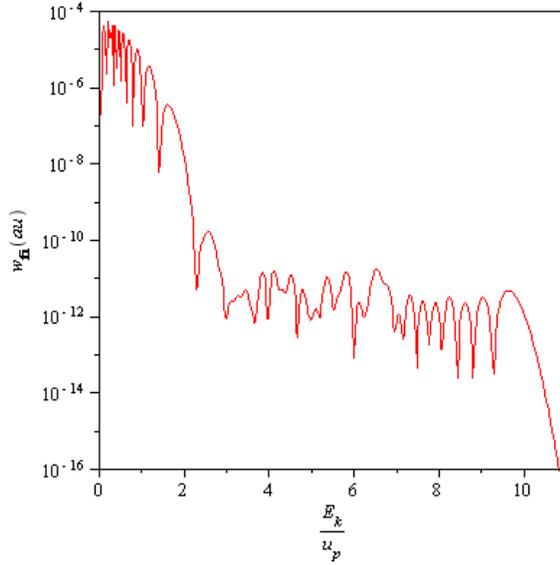


Figure 4.2: Differential ionization rates w_{fi} , in atomic units, of the hydrogen atom as a function of the kinetic energy of electron in units of U_p for $\theta_k = 10^\circ$. The cutoff at $9.6U_p$.

superimposed. From Fig. 4.6 we notice, for the cutoff energy of $10U_p$, that the ionization rate is the largest when $\theta_k = 0^\circ$. For the cutoff energy of $9U_p$, the ionization rate is the largest when $\theta_k = 20^\circ$. For the cutoff energies of $8U_p$ and $6.6U_p$, the ionization rate is the largest when $\theta_k = 30^\circ$, and 40° respectively. Using this, we can explain the appearance of the sidelobes in the high energy part of the spectrum. Thus, the sidelobe for the angle $\theta_k = 10^\circ, 20^\circ, 30^\circ$, and 40° is at $9.6U_p, 9U_p, 8U_p$, and $6.6U_p$ respectively. This means that the angular distributions of the rates for $E_k = 9U_p, 8U_p$, and $6.6U_p$ are elongated along the direction of emission angles of $\theta_k = 20^\circ, 30^\circ$, and 40° respectively.

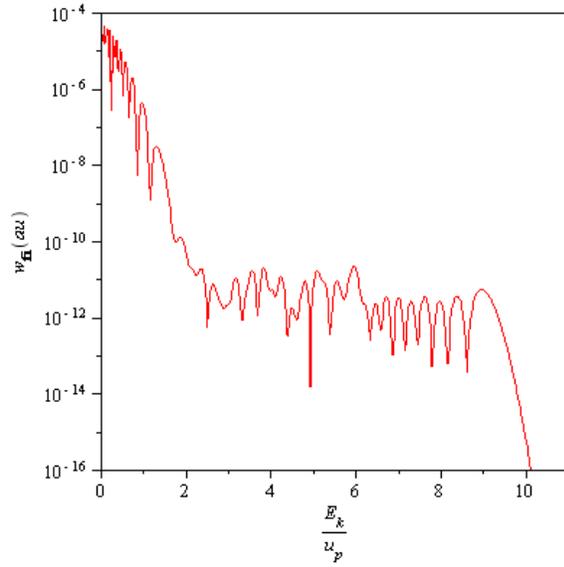


Figure 4.3: Differential ionization rates w_{fi} , in atomic units, of the hydrogen atom as a function of the kinetic energy of electron in units of U_p for $\theta_k = 20^\circ$. The cutoff at $9U_p$.

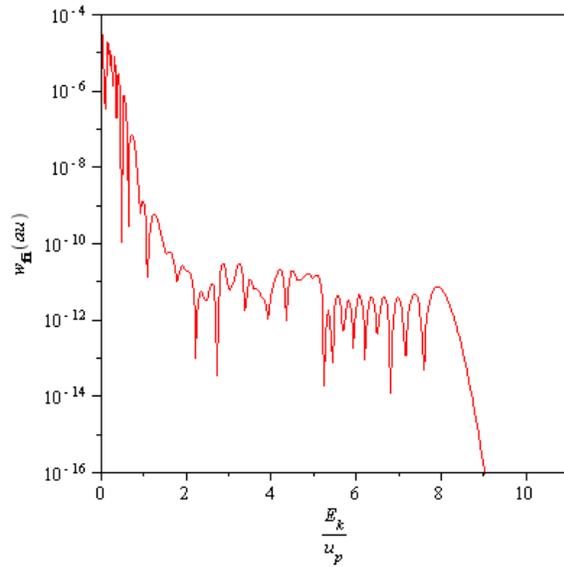


Figure 4.4: Differential ionization rates w_{fi} , in atomic units, of the hydrogen atom as a function of the kinetic energy of electron in units of U_p for $\theta_k = 30^\circ$. The cutoff at $8U_p$.

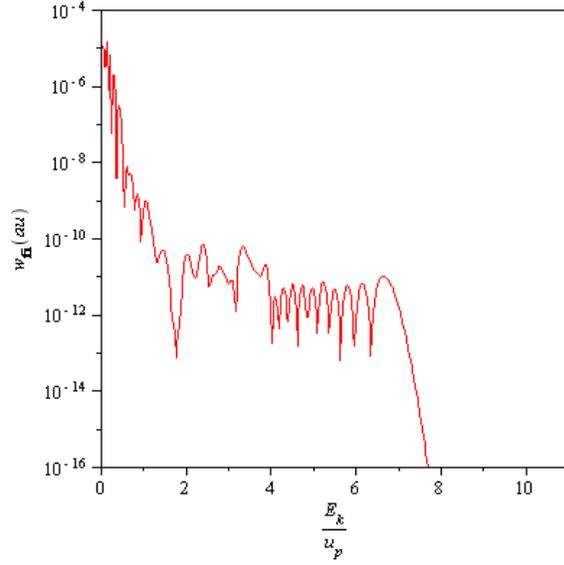


Figure 4.5: Differential ionization rates w_{fi} , in atomic units, of the hydrogen atom as a function of the kinetic energy of electron in units of U_p for $\theta_k = 40^\circ$. The cutoff at $6.6U_p$.

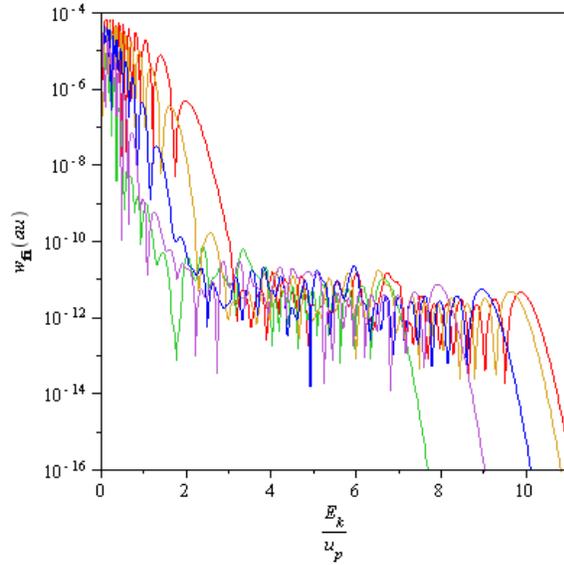


Figure 4.6: Differential ionization rates w_{fi} , in atomic units, of the hydrogen atom as a function of the kinetic energy of electron in units of U_p for $\theta_k = 0^\circ$ red, 10° brown, 20° blue, 30° purple, and 40° green

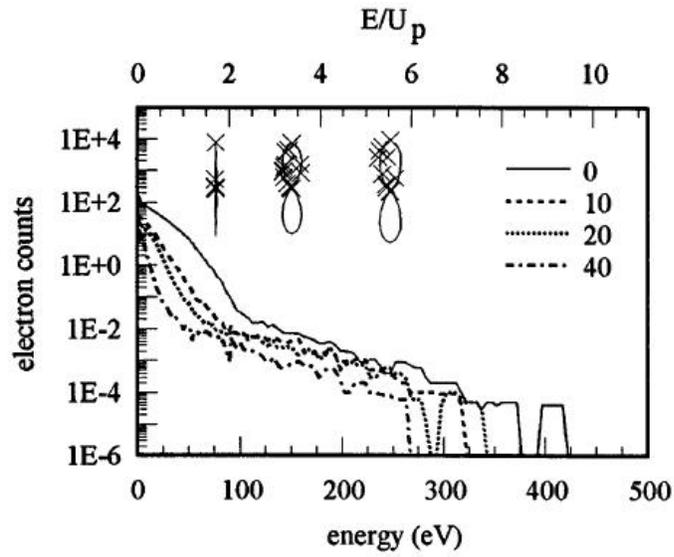


Figure 4.7: Measured helium angle resolved photoelectron spectra for four different emission angles from Walker et al. [13]. The laser parameters are $I = 1.0 \text{ PW/cm}^2$, and $\omega = 1.58 \text{ eV}$. The polar plots show the measured angular distributions (crosses) at the indicated energies and the solid lines are only to guide the reader.

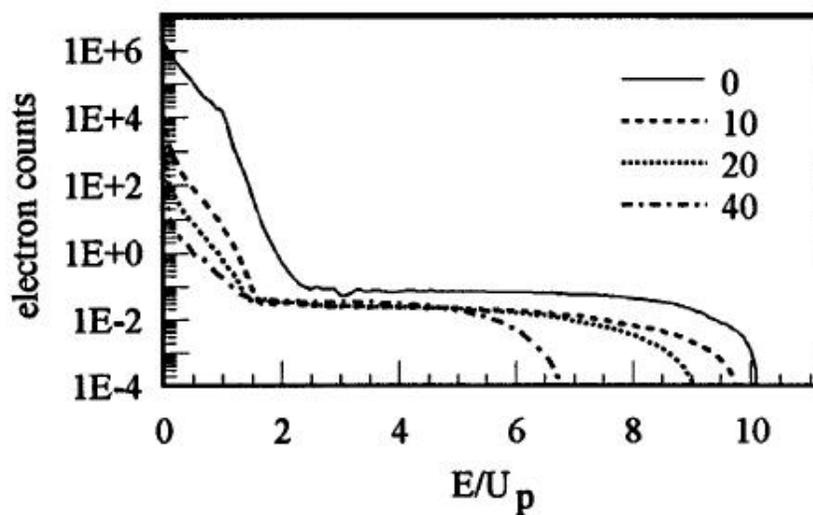


Figure 4.8: Calculated helium angle resolved photoelectron spectra for four different emission angles from Walker et al. [13] using semiclassical theory. The laser parameters are $I = 1.0 \text{ PW/cm}^2$, and $w = 1.58 \text{ eV}$.

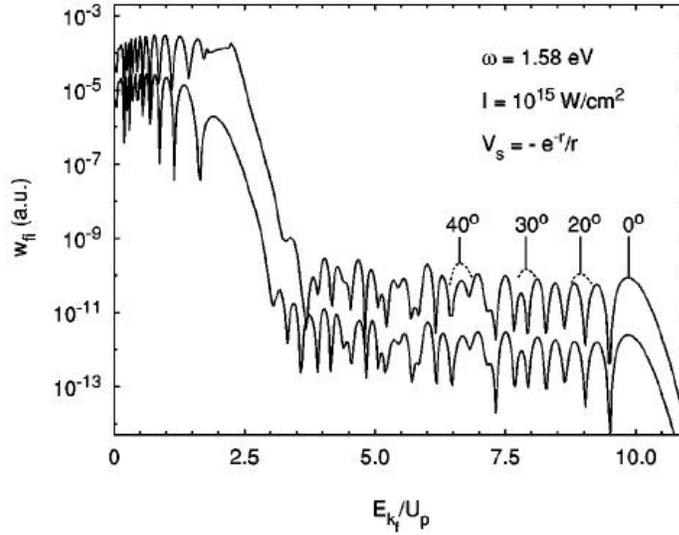


Figure 4.9: Differential ionization rates w_{fi} , in atomic units, of the hydrogen atom as a function of the kinetic energy of electron in units of U_p from Milosevic et al. [59]. The calculations are in the length gauge. The lower curve includes rescattering with no Coulomb effects, while the upper curve includes both the Coulomb and rescattering effects. Both curves correspond to $\theta_k = 0^\circ$. The rounded tops (dotted lines) correspond to the angles $\theta_k = 20^\circ, 30^\circ$, and 40° and the cutoffs are at $9U_p, 8U_p$, and $6.6U_p$ respectively.

Chapter 5

Conclusions

In this dissertation, we have presented a theoretical formulation of above threshold ionization (ATI). We based our formulation utilizing the velocity gauge for the interaction of an atomic system with a strong electromagnetic field rather than the length gauge used nearly in most previous work. The advantage of using the velocity gauge is the ability to carry out more tractable analytical calculations, which in turn leads to more physical insight into the process of ATI. By using the velocity gauge, we were able to develop a detailed *ab initio* formulation of ATI. In the *ab initio* formulation, we demonstrated that the high energy plateau of the photoelectron energy spectrum is due to rescattering by a short range potential (shorter than the Coulomb potential), and the long-range Coulomb potential affects the low energy photoelectrons. Previous analytical attempts [32,33,58,59] to include the effects of the residual ion on the outgoing electron, in order to explain the appearance of the experimentally observed high energy plateau, relied on an *ad hoc model* where it is attributed to a rescattering of the ionized electron at the atomic core. This effect was modeled by a separable short range potential with no long-range Coulomb component at all as in Ref. [33]. In Ref. [32] a zero range potential was considered. Finally, in Refs. [58,59] a more realistic Yukawa potential was considered. They tended to the belief that the short range potential is responsible for the ionized electron rescattering from the atomic core. It is,

therefore, not always present, and may be considered time dependent. Of course the effects of the residual ion on the low energy photoelectron are left out. In our *ab initio* formulation we identify explicitly the short range potential $W(\vec{r}, \vec{\alpha}(t))$ by which the outgoing electron rescatters, giving rise to the experimentally observed high energy plateau. $W(\vec{r}, \vec{\alpha}(t))$ is time dependent and it is present as long as the electromagnetic field is present. Furthermore, unlike the above formulations, we also have demonstrated that only the low energy electrons are affected by the long-range Coulomb potential. Recent experimental findings [78,79], and numerical calculations [80] confirm the effects of the long-range Coulomb potential on the low energy photoelectrons.

Based on the physical insight gained from the *ab initio* approach, we developed an *ad hoc* formulation of ATI, in which we assumed that the influence of the electromagnetic field is to split the atomic potential into two parts: a short range V_s , which is responsible for the high energy plateau, and a long-range Coulomb potential V_c , which affects the low energy electrons which has not been previously included in the velocity gauge. Our use of the Nordseick integrals played a key role in achieving this goal. For the short range potential, V_s , we considered a Yukawa type potential $-Z\frac{e^{-\lambda r}}{r}$ where, for the purpose of accounting for the rescattered electrons of the high energy plateau, the value $\lambda = 1$ is chosen. The results of the numerical calculations which we presented in chapter 4, which are based on this *ad hoc* model, produced an excellent agreement with the findings of Walker et al. [13] and the theoretical calculations of Milosevic et al. [59].

Recent advances in experimental techniques [60,73-75,78-79] allowed the measurement of the low energy one and two dimensional momentum distributions as well as the low energy photoelectron energy distribution. These measurements revealed structures and features that can not be explained within the frame work of the strong field approximation (SFA). Exact solutions of the time dependent Schrödinger equation (TDSE) [61,76,80,81] attributed these structures and features to Coulomb effects only, which as we demonstrated in the *ab initio* formulation, affect the low energy electrons. The SFA assumes for the final state wave function of the outgoing electron a Volkov state solution. This poses no problem for the ATI by a linearly polarized light, since it is associated with no net transfer of angular

momentum. However, it poses a problem for ionization by a circularly polarized electromagnetic field, since the absorption of N photons is associated with a transfer of N units of angular momentum. Of course the recent experimental findings [60,73-75,78-79] and the numerical calculations [61,76,80,81] necessitate the inclusion of the accurate consideration of Coulomb effects in the final state wave function.

In chapter 3, we introduced the final state wave function with accurate consideration of Coulomb effects. This was achieved as a consequence of the most generalized *ab initio* formulation of above threshold ionization which we presented in chapter 3. As a result, by carrying out a partial wave expansion of the final state wave function, we have demonstrated that the absorption of N photons, in the ionization process by a circularly polarized light, is associated with the transfer of N units of angular momentum, and no net transfer of angular momentum, in the ionization process by a linearly polarized light. Again the use of the Nordseick integrals played a key role in reaching this result. Furthermore, using this final wave function, we obtained analytical expressions for the one- and two-dimensional momentum distributions, which are clearly very different from the ones which are based on the SFA. We believe that the recent experimental findings [60,76,80,81] are embedded within these analytical expressions.

Motivated by a private communication with Smeenk et al. [82], we used the final state wave function which we introduced coupled with the inclusion of retardation effects to the long wavelength approximation, and derived an analytical expressions for the ionization rate that include the simultaneous transfer of both linear and angular momenta in the ATI process. Using these ionization rates we obtained an analytical expression for the longitudinal momentum distributions, which clearly show a net longitudinal momentum transfer along the direction of propagation of the electromagnetic field. In the ionization process by a circularly polarized light, a photoelectron is expected to move in the direction of the polarization vector of the field. However, a photoelectron get scattered away from that direction due to the acquired longitudinal momentum along the direction of propagation of the electromagnetic field. This is the ponderomotive scattering. Finally, an expression for the ponderomotive scattering angle, θ_d , which the photoelectron with a final momentum p

makes with the direction of propagation of the electromagnetic field is obtained.

In the body of this dissertation we laid an *ab initio* theoretical understanding of above threshold ionization (ATI). We attribute the newly observed features in the low energy momentum distributions as well as the low energy photoelectron spectrum to be due to *on-shell Coulomb scattering* which is completely absent in the strong field approximation (SFA). Since we have analytically demonstrated in chapter 3 that the high energy photoelectrons are due to *off-shell short range potential scattering*; i.e., population of the essential states, these features are not observed in the high energy photoelectrons.

In the future we will be engaged in a variety of projects –mostly numerical– all stemming from the the analytical formulation laid out in this dissertation:

1. For the first time we will use the short range potential $W(\vec{r}, \vec{\alpha}(t))$ which resulted from the *ab initio* formulation and effectively responsible for the high energy plateau in order to reproduce all experimentally observed features; i.e., a first plateau that extends up to $2U_p$ and a second high energy plateau which extends up to $10U_p$. For this we need an accurate numerical evaluation of Eq. (3.247), which is very similar to Eq. (3.183). In chapter 4 we presented the results of the accurate numerical evaluation of Eq. (3.183). Since Eq. (3.247) is similar to Eq. (3.183) then an accurate numerical evaluation of Eq. (3.247) is achievable.

2. We will carry out an accurate numerical evaluation of Eq. (3.280). In doing so we will be able to confirm - in the case of ionization by a circularly polarized light -the influence of the long-range Coulomb potential on the two dimensional momentum distribution by showing the existence of the counter-intuitive shifts which are observed experimentally by Eckle et al. [60] and predicted numerically by Martiny et al. [61]. We expect to observe these shifts. This is because these shifts are *manifestation of the conservation of angular momentum* which is embedded in Eqs. (3.280) and (3.281).

3. To confirm - in the case of ionization by a linearly polarized light - the role of the Coulomb potential on the low energy momentum distribution along the polarization axis [74] and the low energy photoelectron energy spectrum [79] , an accurate numerical evaluation of Eq. (3.286) is required. In doing so we will be able to confirm that the new features observed in Refs. [74] and [79] are due to *on-shell Coulomb scattering*.

3·By including retardation effects to the long wavelength approximation we arrived at Eqs. (3.351) and (3.353) for the transfer of the longitudinal linear momentum in the ionization process by circularly and linearly polarized light respectively. We argued qualitatively that both of Eqs. (3.351), and (3.353) are not symmetric around the origin of the longitudinal momentum distribution, thus establishing a net transfer of longitudinal momentum and therefore qualitatively agreeing with the findings of Smeenk et al. [82]. To establish a quantitative agreement with Smeenk et al. [82], an accurate numerical evaluation of Eqs. (3.351) and (3.353) is required. Alternatively, we can establish a quantitative agreement with Smeenk et al. [82] by an accurate numerical evaluation of Eqs. (3.368), and (3.372) for both circularly and linearly polarized light respectively.

4·We will accurately evaluate Eq. (3.389) numerically in order to determine with high degree of accuracy the quantum mechanical cutoff for the high harmonic generation (HHG). Eq. (3.389) is mathematically similar to Eq. (3.183) of above threshold ionization (ATI) which we evaluated accurately in Chapter (4).

Appendix A

Nordsieck Type Integrals

Nordsieck type integrals [72,85] I_{ab} appear quite often in atomic collision physics, which is defined as

$$I_{ab} = \int d\vec{r} e^{i(\vec{k}-\vec{k}'-\vec{p})\cdot\vec{r}} \frac{e^{-xr}}{r} {}_1F_1[a, 1, i(kr - \vec{k}\cdot\vec{r})] {}_1F_1[b, 1, i(k'r + \vec{k}'\cdot\vec{r})] \quad (\text{A.1})$$

Using the integral representation [71]

$${}_1F_1[\alpha, \beta; z] = \frac{2^{1-\beta}}{B(\alpha, \beta - \alpha)} e^{z/2} \int_{-1}^1 dt (1-t)^{\beta-\alpha-1} (1+t)^{\alpha-1} e^{\frac{1}{2}zt} \quad (\text{A.2})$$

We obtain

$$\begin{aligned} I_{ab} &= \frac{1}{B(a, 1-a)} \frac{1}{B(b, 1-b)} \int_{-1}^1 dt (1-t)^{-a} (1+t)^{a-1} \int_{-1}^1 du (1-u)^{-b} (1+u)^{b-1} \\ &\times \int d\vec{r} e^{\{\frac{i}{2}[(kr-\vec{k}\cdot\vec{r})t+(k'r+\vec{k}'\cdot\vec{r})u]\}} e^{\{\frac{i}{2}[kr-\vec{k}\cdot\vec{r}+k'r+\vec{k}'\cdot\vec{r}]\}} \frac{e^{-xr}}{r} e^{i(\vec{k}-\vec{k}'-\vec{p})\cdot\vec{r}} \end{aligned} \quad (\text{A.3})$$

Now, if we set

$$\begin{aligned} 2v &= 1+u \\ \lambda &= x - \frac{i}{2}(1+t)k \\ \vec{p}' &= \vec{p} - \frac{1}{2}(1-t)\vec{k} \end{aligned}$$

Then

$$I_{ab} = \frac{1}{B(a, 1-a)} \frac{1}{B(b, 1-b)} \int_{-1}^1 dt (1-t)^{-a} (1+t)^{a-1} \int_0^1 dv (1-v)^{-b} v^{b-1} \\ \times \int d\vec{r} e^{[-\lambda r + ik' vr + i(v\vec{k}' - \vec{k}' - \vec{p}') \cdot \vec{r}]} \frac{1}{r} \quad (\text{A.4})$$

Define

$$\tilde{I} = \int d\vec{r} e^{[-\lambda r + ik' vr + i\vec{Q} \cdot \vec{r}]} \frac{1}{r} \quad (\text{A.5})$$

With

$$\vec{Q} = v\vec{k}' - \vec{k}' - \vec{p}'$$

Then we obtain

$$I_{ab} = \frac{1}{B(a, 1-a)} \frac{1}{B(b, 1-b)} \int_{-1}^1 dt (1-t)^{-a} (1+t)^{a-1} \int_0^1 dv (1-v)^{-b} v^{b-1} \tilde{I} \quad (\text{A.6})$$

The integral \tilde{I} is elementary. Straightforward evaluation gives

$$\tilde{I} = \frac{4\pi}{(-\lambda + ik'v)^2 + Q^2} \quad (\text{A.7})$$

Substituting Eq. (A-7) into Eq. (A-6) gives

$$I_{ab} = \frac{4\pi}{B(a, 1-a)B(b, 1-b)} \int_{-1}^1 dt (1-t)^{-a} (1+t)^{a-1} \int_{-1}^1 du (1-u)^{-b} (1+u)^{b-1} \\ \times \left[\frac{1}{(-\lambda + ik'v)^2 + Q^2} \right] \quad (\text{A.8})$$

Now, if we set

$$v = \frac{1}{1+s} \\ \alpha = (\vec{p}' + \vec{k}')^2 + \lambda^2 \\ \gamma = p'^2 + (\lambda - ik')^2$$

We obtain

$$I_{ab} = \frac{4\pi}{B(a, 1-a)B(b, 1-b)} \int_{-1}^1 dt (1-t)^{-a} (1+t)^{a-1} \frac{1}{\gamma} \int_0^\infty ds \frac{s^{-b}}{[(\alpha/\gamma)s + 1]} \quad (\text{A.9})$$

Since

$$\int_0^\infty dx \frac{x^{\mu-1}}{(1+\beta x)^\nu} = \beta^{-\mu} B(\mu, \nu - \mu) ; |\arg(\beta)| < \pi, \Re(\nu) > \Re(\mu) > 0$$

We have

$$I_{ab} = \frac{4\pi}{B(a, 1-a)} \int_{-1}^1 dt (1-t)^{-a} (1+t)^{a-1} \frac{[\lambda^2 + (\vec{p}' + \vec{k}')^2]^{b-1}}{[p'^2 + (\lambda - ik')^2]^b} \quad (\text{A.10})$$

where we used the property $B(1-b, b) = B(b, 1-b)$. Setting

$$2w = 1 + t$$

And since

$$\begin{aligned} \lambda^2 &= [(x - ik/2) - ikt/2]^2 \\ p'^2 &= [(\vec{p} - \vec{k}/2) + \vec{k}t/2]^2 \\ (\vec{p}' + \vec{k}')^2 &= [(\vec{p} - \vec{k}/2 + \vec{k}') + \vec{k}t/2]^2 \\ (\lambda - ik')^2 &= [(x - ik/2 - ik') - ikt/2]^2 \end{aligned}$$

We obtain

$$I_{ab} = \frac{4\pi}{B(a, 1-a)} \int_0^1 dw w^{a-1} (1-w)^{-a} \frac{\{[x - ikw]^2 + [(\vec{p} - \vec{k} + \vec{k}') + \vec{k}w]^2\}^{b-1}}{\{[(\vec{p} - \vec{k}) + \vec{k}w]^2 + [(x - ik') - ikw]^2\}^b} \quad (\text{A.11})$$

Now if we let

$$\begin{aligned} C &= x^2 + (\vec{p} - \vec{k} + \vec{k}')^2 \\ A &= (x - ik')^2 + (\vec{p} - \vec{k})^2 \end{aligned}$$

so that

$$\begin{aligned} (x - ikw)^2 + [(\vec{p} - \vec{k} + \vec{k}') + \vec{k}w]^2 &= C + 2[\vec{k} \cdot (\vec{p} - \vec{k} + \vec{k}') - ikx]w \\ [(\vec{p} - \vec{k}) + \vec{k}w]^2 + [(x - ik') - ikw]^2 &= A + 2[\vec{k} \cdot (\vec{p} - \vec{k}) - ik(x - ik')]w \end{aligned}$$

therefore,

$$\begin{aligned} I_{ab} &= \frac{4\pi}{B(a, 1-a)} \frac{C^{b-1}}{A^b} \int_0^1 dw w^{a-1} (1-w)^{-a} \left\{ 1 + \frac{2}{c} [\vec{k} \cdot (\vec{p} - \vec{k} + \vec{k}') - ikx] w \right\}^{b-1} \\ &\times \left\{ 1 + \frac{2}{A} [\vec{k} \cdot (\vec{p} - \vec{k}) - ik(x - ik')] w \right\}^{-b} \quad (\text{A.12}) \end{aligned}$$

Since

$$\int_0^1 dx x^{\lambda-1} (1-x)^{\mu-1} (1-ux)^{-\rho} (1-vx)^{-\sigma} = B(\mu, \lambda) F_1[\lambda, \rho, \sigma, \lambda + \mu; u, v]; \Re\lambda > 0, \Re\mu > 0$$

we have

$$I_{ab} = 4\pi \frac{C^{b-1}}{A^b} F_1[a, b, 1-b, 1; -\frac{2}{A}\{\vec{k} \cdot (\vec{p} - \vec{k}) - ik(x - ik')\}, -\frac{2}{C}\{\vec{k} \cdot (\vec{p} - \vec{k} + \vec{k}') - ikx\}] \quad (\text{A.13})$$

Utilizing

$$F_1[\alpha, \beta, \beta', \beta + \beta'; u, v] = (1-v)^{-\alpha} {}_2F_1[\alpha, \beta, \beta + \beta'; \frac{u-v}{1-v}]$$

and setting

$$\begin{aligned} u &= -\frac{2}{A}\{\vec{k} \cdot (\vec{p} - \vec{k}) - ik(x - ik')\} \\ v &= -\frac{2}{C}\{\vec{k} \cdot (\vec{p} - \vec{k} + \vec{k}') - ikx\} \\ Y &= \frac{u-v}{1-v} \end{aligned}$$

we finally obtain

$$I_{ab} = 4\pi \frac{C^{a+b-1}}{A^b B^a} {}_2F_1[a, b, 1, Y] \quad (\text{A.14})$$

where,

$$\begin{aligned} A &= (x - ik')^2 + (\vec{p} - \vec{k})^2 \\ B &= (x - ik)^2 + (\vec{p} + \vec{k}')^2 \\ C &= x^2 + (\vec{p} - \vec{k} + \vec{k}')^2 \\ Y &= \frac{2}{AB} \left\{ A[\vec{k} \cdot (\vec{p} - \vec{k} + \vec{k}') - ikx] - C[\vec{p} \cdot k - k^2 - ikx - kk'] \right\} \end{aligned}$$

Appendix B

Saddle-Point Method

The saddle-point method is applicable, in general, to integrals of the form

$$I(s) = \int_C dz g(z) e^{sf(z)} \quad (s \text{ is large and positive}) \quad (\text{B.1})$$

where C is a path in the complex plane such that the ends of the path do not contribute significantly to the integral. It is further assumed that the factor $g(z)$ in the integrand is dominated by the exponential in the region of interest. Since s is large and positive, the value of the integrand will become large when the real part of $f(z)$ is large and small when the real part of $f(z)$ is small or negative. In particular, as s is permitted to increase indefinitely, the entire contribution of the the integrand to the integral will come from the region in which the real part of $f(z)$ takes on a positive maximum value. A way from this positive maximum the integrand will become negligibly small in comparison. Now we write

$$f(z) = u(x, u) + v(x, u) \quad (\text{B.2})$$

If now, in addition, we impose the condition that the imaginary part $v(x, y)$ of $f(z)$ to be constant, that is, $v(x, y) = v_0$, we may approximate the integral by

$$I(s) \approx e^{w_0} \int_C dz g(z) e^{su(x,y)} \quad (\text{B.3})$$

A way from the maximum of the real part, the imaginary part may be permitted to oscillate as it wishes, for the integrand is negligibly small and the varying phase factor is therefore irrelevant. Since $f(z)$ is a continuous function, it satisfies Cauchy-Riemann equations and therefore $\nabla^2 u = 0$ and $\nabla^2 v = 0$. Consequently neither u nor v can have a maximum or minimum except at a singularity. For example, if

$$\frac{\partial^2 u}{\partial x^2} < 0 \text{ then } \frac{\partial^2 u}{\partial y^2} > 0$$

so that a "flat spot" on the surface $u(x, y)$, where

$$\frac{\partial u}{\partial x} = \frac{\partial u}{\partial y} = 0 \tag{B.4}$$

must be a "saddle point," where the surface looks like a saddle or a mountain pass. By the Cauchy-Riemann Equations, we see that Eq. (B.4) implies $\frac{\partial v}{\partial y} = 0$ and $\frac{\partial v}{\partial x} = 0$, so that $f'(z) = 0$. Thus a saddle point of the function $u(x, y)$ is also a saddle point of $v(x, y)$ as well as a point where $f'(z) = 0$.

near the saddle point z_0 ,

$$f(z) \approx f(z_0) + \frac{1}{2}f''(z_0)(z - z_0)^2 \tag{B.5}$$

The term $\frac{1}{2}f''(z_0)(z - z_0)^2$, is real and negative. It is real, for we have specified that the imaginary part shall be constant along our contour and negative because we are moving down from the saddle point or mountain pass (at the saddle point z_0 , $u(x, y)$ has a maximum). Assuming $f''(z_0) \neq 0$, we write

$$\frac{1}{2}f''(z_0)(z - z_0)^2 = -\frac{1}{2s}t^2 \tag{B.6}$$

Also

$$(z - z_0) = \delta e^{i\alpha} \text{ } (\alpha \text{ held constant}) \tag{B.7}$$

Therefore we have

$$t^2 = -s f''(z_0) \delta^2 e^{2i\alpha} \tag{B.8}$$

Since t is real, it may be written

$$t = \pm \delta |s f''(z_0)|^{\frac{1}{2}} \tag{B.9}$$

Substituting into Eq. (B.1), we obtain

$$I(s) \approx g(z_0)e^{sf(z_0)} \int_{-\infty}^{\infty} e^{-\frac{t^2}{2}} \frac{dz}{dt} dt \quad (\text{B.10})$$

where, the limits of integration is extended to $\pm\infty$, for the integrand is negligible as we move down from the saddle point. Since

$$\frac{dz}{dt} = |sf''(z_0)|^{-\frac{1}{2}} e^{i\alpha} \quad (\text{B.11})$$

we finally obtain

$$I(s) \approx \frac{\sqrt{2\pi}g(z_0)e^{sf(z_0)}e^{i\alpha}}{|sf''(z_0)|^{\frac{1}{2}}} \quad (\text{B.12})$$

The phase α is chosen so that the two conditions given [α is constant; real part of $f(z)$ has a maximum at the saddle point z_0] are satisfied.

The same approach can be generalized to integrals of the form

$$I(t) = \int d\vec{q} h(\vec{q}) e^{-iS[\vec{q};t]} \quad (\text{B.13})$$

where $S[\vec{q}; t]$, is a real function of \vec{q} and t is a parameter, for example time. We assume the factor $h(\vec{q})$ is dominated by the exponential in the region of interest. When $S[\vec{q}; t] \gg 1$, most of the contribution to the integral comes from a small region in the vicinity of the saddle point \vec{q}_s , where $S[\vec{q}_s]$ has a maximum. As we move away from the saddle point, the integrand oscillates so many times resulting in cancelation of contributions of the integrand outside the region of interest. At the saddle point \vec{q}_s , $S[\vec{q}; t]$ is stationary. Since $S[\vec{q}; t]$ has no imaginary part, the method is called in this case " the stationary phase method". The condition for $S[\vec{q}; t]$ to be stationary is

$$\vec{\nabla}_{\vec{q}} S[\vec{q}; t] = 0 \quad (\text{B.14})$$

Near the saddle point \vec{q}_s ,

$$S[\vec{q}; t] \approx S[\vec{q}_s; t] + \left\{ \frac{1}{2} \frac{\partial^2}{\partial \vec{q}^2} S[\vec{q}; t] \right\}_{\vec{q}=\vec{q}_s} (\vec{q} - \vec{q}_s)^2 \quad (\text{B.15})$$

Setting $\vec{p} = \vec{q} - \vec{q}_s$ and substituting Eq. (B.15) into Eq. (B.13) we obtain

$$I(t) \approx h(\vec{q}_s) e^{-iS[\vec{q}_s; t]} \int d\vec{p} e^{-i \left\{ \frac{1}{2} \frac{\partial^2}{\partial \vec{q}^2} S[\vec{q}; t] \right\}_{\vec{q}=\vec{q}_s} p^2} \quad (\text{B.16})$$

The integral over \vec{p} is straightforward and so we finally obtain

$$I(t) \approx h(\vec{q}_s) e^{-\iota S[\vec{q}_s; t]} \left(\frac{2\pi}{\iota \left\{ \frac{\partial^2}{\partial \vec{q}^2} S[\vec{q}; t] \right\}_{\vec{q}=\vec{q}_s}} \right)^{\frac{3}{2}} \quad (\text{B.17})$$

For an electron inside electromagnetic field, $S[\vec{q}; t, \tau]$ is the semiclassical action which is given by

$$S[\vec{q}; t, \tau] = \frac{1}{2} \int dt' [\vec{q} + \frac{1}{c} \vec{A}(t')]^2 \quad (\text{B.18})$$

Therefore

$$\begin{aligned} \vec{q}_s &= \frac{1}{\tau} [\vec{\alpha}(t - \tau) - \vec{\alpha}(t)] \\ \tau &= \left\{ \frac{\partial^2}{\partial \vec{q}^2} S[\vec{q}; t] \right\}_{\vec{q}=\vec{q}_s} \end{aligned}$$

where $\vec{\alpha}$ is given by

$$\vec{\alpha}(t) = \frac{1}{c} \int^t dt' \vec{A}(t')$$

Appendix C

Numerical Integration Methods

Before we outline the Fourier transform method and the double exponential method, we prelude to the Euler-Maclaurin summation formula.

C.1 Euler-Maclaurin Summation Formula

If $g(x)$ is $(2k + 1)$ continuous function, then we state with no proof Euler-Maclaurin summation formula (for proof see Ref. [86])

$$\int_a^b g(x)dx - T_n(g) = \sum_{j=1}^k \frac{B_{2j}}{(2j)!} h^{2j} [g^{(2j-1)}(b) - g^{(2j-1)}(a)] - h^{2k+1} \int_a^b P_{2k+1}\left(n \frac{x-a}{x-b}\right) g^{(2k+1)}(x) dx \quad (\text{C.1})$$

where $h = (b-a)/n$ and the constants B_{2j} are the Bernoulli numbers. $P_{2k+1}(x)$ is a periodic function of x ,

$$P_{2k+1}(x) = (-1)^{k-1} \sum_{j=1}^{\infty} \frac{2 \sin(2\pi j x)}{(2\pi j)^{2k+1}} \quad (\text{C.2})$$

and $T_n(g)$ designates the trapezoidal sum,

$$T_n(g) = h \left[\frac{1}{2} g(a) + g(a+h) + g(a+2h) + \dots + g(a+(n-1)h) + \frac{1}{2} g(b) \right] \quad (\text{C.3})$$

Thus, the right hand side of Eq. (C.1) is the error in approximating the integral $\int_a^b g(x)dx$ by the trapezoidal sum $T_n(g)$.

Now, let assume that $g^{(2j-1)}(a) = g^{(2j-1)}(b)$ and let $|g^{2k+1}(x)| \leq M$ for $a \leq x \leq b$. From Eq. (C.2) we have

$$|P_{2k+1}(x)| = |(-1)^{k-1} \sum_{j=1}^{\infty} \frac{2 \sin(2\pi jx)}{(2\pi j)^{2k+1}}| \leq \sum_{j=1}^{\infty} \frac{2}{(2\pi j)^{2k+1}} = 2^{-2k} \pi^{-2k-1} \zeta(2k+1). \quad (\text{C.4})$$

where $\zeta(k) = \sum_{j=1}^{\infty} j^{-k}$ is the Reimann zeta function.

Therefore from Eq. (C.1) we have

$$|\int_a^b g(x)dx - T_n| \leq h^{2k+1} \int_a^b |P_{2k+1}(n \frac{x-a}{x-b})| |g^{(2k+1)}| dx \quad (\text{C.5})$$

Utilizing Eq. (C.4) we obtain

$$|\int_a^b g(x)dx - T_n| \leq \frac{C}{n^{2k+1}} \quad (\text{C.6})$$

the constant C is finite and independent of n and is taken to be

$$C = M(b-a)^{2k+2} 2^{-2k} \pi^{-2k-1} \zeta(2k+1)$$

Thus for rapid convergence with the trapezoidal rule it is sufficient to have a function $g(x)$ for which $g'(a) = g'(b), g''(a) = g''(b), g'''(a) = g'''(b)$, and so on. A periodic function with period $b-a$ which is $(2k+1)$ continuous over $[-\infty, \infty]$ is such a function.

C.2 Fourier Transform Method

If $h(t)$ is a smooth well behaved function over the interval $[-\infty, \infty]$ then its Fourier transform $H(\omega)$ is

$$H(\omega) = \int_{-\infty}^{\infty} h(t) e^{i\omega t} dt \quad (\text{C.7})$$

and the inverse Fourier Transform is

$$h(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} H(\omega) e^{-i\omega t} d\omega \quad (\text{C.8})$$

In most common situations, the function $h(t)$ is sampled (i.e its value is recorded) at evenly intervals in t . The objective is to estimate the Fourier transform of $h(t)$ from a finite number of its sampled points. Suppose that we have N consecutive sampled values

$$h_k \equiv h(t_k), \quad t_k \equiv k\Delta, \quad k = 0, 1, 2, \dots, N - 1 \quad (\text{C.9})$$

so that the sampling interval is Δ . The sampling procedure and thus the sampled points are supposed to be at least typical of what $h(t)$ looks like at all t .

With N numbers of input, we will evidently be able to produce no more than N independent numbers of output. So, instead of trying to estimate the Fourier transform $H(\omega)$ at all values of ω , let us seek estimates at discrete values

$$\omega_n = \frac{2\pi n}{N\Delta}, \quad n = -\frac{N}{2}, \dots, \frac{N}{2} \quad (\text{C.10})$$

where for simplicity N is taken to be even. The remaining step is to approximate the integral in Eq. (C.7) by a discrete sum:

$$H(\omega_n) = \int_{-\infty}^{\infty} h(t) e^{i\omega_n t} dt \approx \sum_{k=0}^{N-1} h_k e^{i\omega_n t_k} \Delta = \Delta \sum_{k=0}^{N-1} h_k e^{2\pi i k n / N} \quad (\text{C.11})$$

The final summation in Eq. (C.11) is called the *discrete Fourier transform* (DFT) of the N points h_k [87,88]. Let us denote it by H_n ,

$$H_n \equiv \sum_{k=0}^{N-1} h_k e^{2\pi i k n / N} \quad (\text{C.12})$$

The discrete Fourier transform maps N complex numbers (the h_k 's) into N complex numbers (the H_n 's). The relation (C.11) between the discrete Fourier transform of a set of numbers and their continuous Fourier transform when they are viewed as samples of a continuous function sampled at interval Δ can be rewritten as

$$H(\omega_n) \approx \Delta H_n \quad (\text{C.13})$$

where ω_n is given by Eq. (C.10).

For any sampling interval Δ , there is a special frequency ω_c , called the *Nyquist critical frequency*, given by

$$\omega_c \equiv \frac{\pi}{\Delta} \quad (\text{C.14})$$

Since $t_k = k\Delta$ then it is readily seen from Eq. (C.11) that two discrete frequencies ω_n and $\omega_{n'}$ give the same samples at an interval Δ if ω_n and $\omega_{n'}$ differ by a multiple of $\frac{2\pi}{\Delta}$, which is just the width in frequency of the range $(-\omega_c, \omega_c)$. This means that for a given interval Δ , sampling a continuous function that is bandwidth limited to less than the Nyquist critical frequency, i.e. $-\omega_c < \omega_n < \omega_c$, poses no problem. However, any frequency component ω_n outside of the frequency range $(-\omega_c, \omega_c)$ is spuriously moved (falsely translated) into that range by the very act of discrete sampling. This is called *aliasing*. To overcome aliasing one need to (i) know the natural bandwidth limit of the signal, and then (ii) sample at a rate sufficiently rapid to give at least two points per cycle of the highest frequency present. (i.e, for any sampling interval Δ , we come to estimate the Fourier transform of a continuous function from the discrete samples at the discrete frequencies ω_n that lie in the range $(-\omega_c, \omega_c)$.)

It easily seen from Eq. (C.12) that H_n is periodic in n , with period N . Therefore $H_{-n} = H_{N-n}$ $n = 1, 2, \dots$. With this conversion in mind one generally lets n in H_n vary from 0 to $N - 1$. Then n and k in (h_k) vary exactly over the same range, manifesting the mapping of N numbers into N numbers. With this convention in mind, one must remember that zero frequency corresponds to $n = 0$, positive frequencies $0 < \omega_n < \omega_c$ correspond to values $1 \leq n \leq N/2 - 1$, while negative frequencies $-\omega_c < \omega_n < 0$ correspond to $N/2 + 1 \leq n \leq N - 1$. The value $n = N/2$ corresponds to both $\pm\omega_c$.

How much computation is involved in computing the discrete Fourier transform (C.12) of N points? If we define the complex number $W \equiv e^{2\pi i/N}$ then Eq. (C.12) becomes

$$H_n = \sum_{k=0}^{N-1} W^{nk} h_k \tag{C.15}$$

Thus, the column vector H is the product of the matrix W , of order $(N \times N)$, multiplied by the column vector h . So, the DFT appears to be an $O(N^2)$ process. This is deceiving. In fact the DFT can be computed in $O(N \log_2 N)$ operations with a procedure called the fast Fourier transform (FFT). With large $N = 10^6$, for example, the difference between N^2 and $N \log_2 N$ is immense. The idea behind the FFT is the fact that a DFT of length N can be written as the sum of two DFT, each of length $N/2$. One is formed from the even-numbered

points of the the original N , the other from the odd-numbered points. To see this we write

$$\begin{aligned}
 H_n &= \sum_{k=0}^{N-1} e^{2\pi i n k / N} h_k \\
 &= \sum_{k=0}^{N/2-1} e^{2\pi i n (2k) / N} h_{2k} + \sum_{k=0}^{N/2-1} e^{2\pi i n (2k+1) / N} h_{2k+1} \\
 &= \sum_{k=0}^{N/2-1} e^{2\pi i n k / (N/2)} h_{2k} + W^n \sum_{k=0}^{N/2-1} e^{2\pi i n k / (N/2)} h_{2k+1} \\
 &= H_n^e + W^n H_n^o
 \end{aligned} \tag{C.16}$$

where H_n^e denotes the n th component of the fourier transform of length $N/2$ formed from the even components of the original h_k 's, while H_n^o is the corresponding transformation of length $N/2$ formed from the odd components. This procedure is applied again to H_n^e and H_n^o resulting in the four Fourier transforms H_n^{ee} , H_n^{eo} , H_n^{oo} and H_n^{oe} , each of length $N/4$. Provide that $N = 2^\nu$, where ν is an integer, then we can continue applying this procedure until we have subdivided the data all the way down to transforms of length 1. The Fourier transform of input data of length 1 is itself. In other words, for an input data of length $N = 2^\nu$, there is $\nu = \log_2 N$ subdivisions, resulting in $\log_2 N$ pattern of e 's and o 's. For each pattern of $\log_2 N$ e 's and o 's there is a one-point transform that is just one of the input numbers h_k

$$H_n^{eoeoeo\dots oee} = h_k \text{ for some } k = 0, 1, \dots, N - 1 \tag{C.17}$$

The next question is: which value of k corresponds to which pattern of e 's and o 's? We can get insight to answer this question by taking, for example, a set of $N = 16 = 2^4$ data points $h_0, h_1, h_2, \dots, h_{15}$. Consider a specific pattern of $\nu = 4$ e 's and o 's, say H^{eoeo} . According to this pattern, after the first subdivision, H^e , we retain the 8 even data points $h_0, h_2, h_4, h_6, h_8, h_{10}, h_{12}, h_{14}$. The new set of 8 data points is to be subdivided (second subdivision H^{eo}) retaining only the 4 odd data points h_2, h_6, h_{10}, h_{14} . The third subdivision, H^{eoe} , retains only the 2 even data points h_2, h_{10} . The final subdivision, H^{eoeo} , result in the one point transform h_{10} . Thus $H^{eoeo} = h_{10}$. In binary representation, $10 = 1010$. If we let $e = 0$ and $o = 1$, then the pattern $eoeo = 0101$, which is the bit reversed representation

of 10. Thus reverse the pattern of $eoeo$ to $oeoe$ then we have the binary representation $1010 = 10$. Guided by this insight, we can now answer the above question: For any pattern of $\log_2 N$ e's and o's, reverse the pattern of e's and o's then let $e = 0$ and $o = 1$, and you will have in binary the value of k . So take the original set of $N = 2^\nu$ data points h_k and rearrange it into bit-reversed order, so that the individual numbers are in order not of k , but of the number obtained by bit-reversing k . Then, the points as given are the one-point transforms. Combine adjacent pairs to get two two-point transforms, then combine adjacent pairs of pairs to get 4-point transforms, and so on, until the first and second halves of the whole data set are combined into the the final transform. Each combination takes of order N operations, and there are evidently $\nu = \log_2 N$ combinations, so that the whole FFT procedure is of the order $N \log_2 N$ (of course, the process of rearranging original data into bit-reversed order is of the order of $N \log_2 N$).

C.2.1 Computing Fourier Components

Of interest in this work is to calculate accurately the numerical values of the Fourier components $I(n)$,

$$I(n) = \int_0^{2\pi} h(t) e^{int} dt \quad (\text{C.18})$$

where $h(t)$ is periodic function with period 2π and n is an integer. In general, one wants to evaluate $I(n)$ for many different values of n . Without any loss of generality we evaluate $I(\omega)$,

$$I(\omega) = \int_a^b h(t) e^{i\omega t} dt \quad (\text{C.19})$$

where $h(t)$ is not necessarily periodic. It is intuitively obvious that the Fourier transform method ought to be applicable to this problem. Divide the interval $[a, b]$ into M subintervals, where M is large integer, and define

$$\Delta \equiv \frac{b-a}{M}, \quad t_j \equiv a + j\Delta, \quad h_j \equiv h(t_j), \quad j = 0, 1, \dots, M \quad (\text{C.20})$$

In particular, we can choose M to an integer power of 2, and define a set of special ω 's by

$$\omega_n \Delta \equiv \frac{2\pi n}{M} \quad (\text{C.21})$$

where $n = 0, 1, \dots, M/2 - 1$. Then the integral $I(\omega)$ is approximated as

$$I(\omega_n) \approx \Delta e^{i\omega_n a} \sum_{j=0}^{M-1} h_j e^{2\pi n j / M} = \Delta e^{i\omega_n a} [DFT(h_0 \dots h_{M-1})]_n \quad (\text{C.22})$$

When $[a, b] \equiv [0, 2\pi]$ then $\omega_n = n$ therefore, $I(\omega_n) \equiv I(n)$ for a periodic $h(t)$. For a given $\omega_n = n$, the integrand $h(t)e^{i\omega_n t}$ is periodic. Therefore the DFT becomes trapezoidal sum which for periodic functions, as we shown in the beginning of this appendix, converges rapidly with high degree of accuracy.

When function $h(t)$ is not periodic, Eq. (C.22) must be modified to include correction terms. A more sophisticated treatment is required. Given the sampled points h_j , we can approximate the function $h(t)$ everywhere in the interval $[a, b]$ by interpolation on nearby h_j 's. The simplest case is linear interpolation, using the two nearest h_j 's, one to left and one to the right. In general, the formulas for such interpolation schemes are piecewise polynomial (called kernel) in the independent variable t , but with coefficients that are of course linear in the function values h_j . Thus we write

$$h(t) \approx \sum_{j=0}^M h_j \psi\left(\frac{t-t_j}{\Delta}\right) + \sum_{j=\text{endpoints}} h_j \varphi_j\left(\frac{t-t_j}{\Delta}\right) \quad (\text{C.23})$$

Here $\psi(s)$ is the kernel function of an interior point: it is zero for s sufficiently negative or sufficiently positive, and becomes nonzero only when s is in the range where the h_j multiplying it is actually used in the interpolation. We always have $\psi(0) = 1$ and $\psi(m) = 0, m = \pm 1, \pm 2, \dots$, since interpolation right on a sample point should give the sampled function value. $\varphi_j(s)$ is the kernel function of an endpoint, reflecting the fact that subintervals closest to a and b require different (noncentered) interpolation formulas.

Now apply the integral operator $\int_a^b dt e^{i\omega t}$ to both sides of Eq. (C.23), interchange the sums and the integral, and make the changes of variable $s = (t - t_j)/\Delta$ in the first sum, $s = (t - a)/\Delta$ in the second sum. The result is

$$I \approx \Delta e^{i\omega a} \left[W(\theta) \sum_{j=0}^M h_j e^{i j \theta} + \sum_{j=\text{endpoints}} h_j \alpha_j(\theta) \right] \quad (\text{C.24})$$

Here $\theta \equiv \omega \Delta$, and the functions $W(\theta)$ and $\alpha_j(\theta)$ are defined by

$$W(\theta) = \int_{-\infty}^{\infty} ds e^{i\theta s} \psi(s) \quad (\text{C.25})$$

$$\alpha_j(\theta) = \int_{-\infty}^{\infty} ds e^{i\theta s} \varphi(s-j) \quad (\text{C.26})$$

Eqs. (C.25) and (C.26) can be evaluated, analytically, for any given interpolation scheme. Then Eq. (C.24) contains endpoint corrections to a sum which can be done using Fourier transform method, giving a result with high-order accuracy.

Imposing left-right symmetry on interpolation we have

$$\varphi_{M-j}(s) = \varphi_j(-s), \quad \psi(s) = \psi(-s), \quad \alpha_{M-j}(\theta) = e^{i\theta M} \alpha_j^*(\theta) = e^{i\omega(b-a)} \alpha_j^*(\theta) \quad (\text{C.27})$$

We consider only linear (trapezoidal order) interpolation. In this case $\psi(s)$ is a piecewise linear, rises from 0 to 1 for s in $(-1, 0)$, and falls back to 0 for S in $(0, 1)$ and from the symmetry relations (C.27), $W(\theta)$, α_M are evaluated to be

$$W(\theta) = \frac{2(1 - \cos \theta)}{\theta^2} \quad (\text{C.28})$$

$$\alpha_0 = -\frac{(1 - \cos \theta)}{\theta^2} + i \frac{(\theta - \sin \theta)}{\theta^2} \quad (\text{C.29})$$

$$\alpha_M(\theta) = e^{i\omega(b-a)} \alpha_0^*(\theta) \quad (\text{C.30})$$

Now, for ω_n satisfying Eq. (C.21) we have

$$I(\omega_n) = \Delta e^{i\omega_n a} \{W(\theta)[DFT(h_0 \dots h_{M-1})]_n + \alpha_0(\theta)h_0 + e^{i\omega(b-a)\alpha_0^*(\theta)h_M}\} \quad (\text{C.31})$$

When $h(t)$ is periodic, then $h(a) = h(b)$, and therefore Eq. (C.31) reduces to Eq. (C.22).

C.3 The Double Exponential Method

The double exponential method (DEM) method evaluates integrals with end-point singularity efficiently which conventional methods often fail to do. It is based on the double exponential transformation (DET) in the following manner. Given an integral

$$I = \int_a^b f(x)dx, \quad (\text{C.32})$$

where $f(x)$ is analytic function on (a, b) with the possibility of being singular at $x = a$ or $x = b$ or both as long as I is integrable. If we carry a variable transformation such that

$$x = \phi(t), \quad \phi(-\infty) = a \quad \phi(\infty) = b \quad (\text{C.33})$$

to obtain

$$I = \int_{-\infty}^{\infty} f(\phi(t))\phi'(t) dt \quad (\text{C.34})$$

In addition, we impose a property to $\phi(t)$ such that $\phi'(t)$ tends to 0 double exponentially as $t \rightarrow \pm\infty$, i.e.

$$|\phi'(t)| \rightarrow e^{-ce^{|t|}} \text{ as } t \rightarrow \pm\infty \quad (\text{C.35})$$

Next, we apply the trapezoidal rule with an equal mesh size to get

$$I_h = h \sum_{n=-\infty}^{\infty} f(\phi(nh))\phi'(nh) \quad (\text{C.36})$$

In actual computation we must truncate the summation at some $n = -N_-$ and $+N_+$, i.e

$$I_h^{(N)} = h \sum_{n=-N_-}^{N_+} f(\phi(nh))\phi'(nh), \quad N = N_- + N_+ + 1 \quad (\text{C.37})$$

where N is the total number of function evaluations. Since $\phi'(nh)$ and hence $f(\phi(nh))\phi'(nh)$, decays double exponentially at large $|n|$, we call the quadrature formula (C.37) a DE formula. Even if $f(x)$ is singular at $x = a$ or $x = b$, integral (C.34) is integrable as long as (C.32) integrable, and we can truncate the summation (C.37) at moderate $n = -N_-$ and N_+ .

Now, consider the contour integral, J ,

$$J = \int_C \frac{f(\phi(w))\phi'(w)}{1 - e^{-2\pi w/h}} dw \quad (\text{C.38})$$

where C is a closed contour in the complex w -plane which runs from left to right along the real axis and returns above the real axis from right to left. Moreover, C is chosen such that the singularities of $f(\phi(w))\phi'(w)$ lie outside C . There are simple poles at $w = nh$ and If C' is the portion of C that runs from right to left above the real axis, then we have

$$\begin{aligned} J &= I + \int_{C'} \frac{f(\phi(w))\phi'(w)}{1 - e^{-2\pi w/h}} dw \\ &= 2\pi i \sum \text{Res}|_{w=nh} = h \sum_{n=-\infty}^{\infty} f(\phi(nh))\phi'(nh) \end{aligned}$$

therefore, the error of I_h due to the trapezoidal sum, ΔI_h , which is called the discretization error, is given by

$$\Delta_h = I - I_h = \int_{C'} \frac{f(\phi(w))\phi'(w)}{e^{-2\pi w/h} - 1} dw \quad (\text{C.39})$$

The contour integral over C' can be cast into a form suitable to be evaluated using the saddle point method (see appendix B). Takahashi et al. [67] have shown that

$$|\Delta I_h| \approx B e^{-A/h} \quad (\text{C.40})$$

where A is a constant depending of the distance of the nearest saddle points of $|\frac{f(\phi(w))\phi'(w)}{e^{-2\pi i w/h}-1}|$ to the real axis and B is also a constant depending on the magnitude of the integral I itself.

C.3.1 DE Formula For Oscillatory Integrals

We consider the following integrals

$$I_s = \int_0^\infty f(x) \sin \omega x dx \quad (\text{C.41})$$

$$I_c = \int_0^\infty f(x) \cos \omega x dx \quad (\text{C.42})$$

where, $f(x)$ is assumed to converge very slowly as $x \rightarrow \infty$ ($f(x)$ can be oscillatory too) and ω is a parameter which, without loss of generality, is taken to be positive. We will outline the method for the integral I_s .

We carry a variable transformation

$$x = M\varphi(t)/\omega, \quad \varphi(t) = \frac{t}{1 - \exp(-2t - \alpha(1 - e^{-t}) - \beta(e^t - 1))} \quad (\text{C.43})$$

and obtain

$$I = \int_{-\infty}^\infty f(M\varphi(t)/\omega) \sin(M\varphi(t))(M/\omega)\varphi'(t)dt \quad (\text{C.44})$$

where M , α and β are positive constants (see Refs [67,68])

$$\beta = 1/4, \quad \alpha = \beta/\sqrt{1 + M \ln(1 + M)/4\pi}$$

and M to be determined latter. Applying the trapezoidal rule with mesh size h , we have

$$I_{s,h} = \frac{Mh}{\omega} \sum_{n=-\infty}^\infty f\left(\frac{M}{\omega}\varphi(nh)\right) \sin(M\varphi(nh))\varphi'(nh) \quad (\text{C.45})$$

as n becomes large and negative, the summand decays double exponentially (due to $\varphi'(nh)$) . If M is chosen to satisfy $Mh = \pi$ then, $\sin(M\varphi(nh)) \rightarrow \sin(n\pi) = 0$ rapidly as $n \rightarrow \infty$

since $\varphi(t)/t \rightarrow 1$ as $t \rightarrow \infty$, and therefore $I_{s,h}$ converges to I very quickly. The summation can be truncated at moderate $n = -N_-$ and N_+ so that

$$I_{s,h}^{(N)} = \frac{Mh}{\omega} \sum_{n=-N_-}^{N_+} f\left(\frac{M}{\omega}\varphi(nh)\right) \sin(M\varphi(nh))\varphi'(nh), \quad Mh = \pi \quad (\text{C.46})$$

where $N = N_- + N_+ + 1$ is the number of function evaluations. The error is bounded as

$$|I - I_{s,h}^{(N)}| < c' e^{-c/h} \quad (\text{C.47})$$

where c and c' are positive constants depending only on $f(x)$ and ω .

For the I_c integral we use

$$x = M\varphi\left(t - \frac{\pi}{2M}\right)/\omega \quad (\text{C.48})$$

where $\varphi(t)$ is given by Eq. (C.43). Then, if we require $Mh = \pi$, we have

$$I_{c,h}^{(N)} = \frac{Mh}{\omega} \sum_{n=-N_-}^{N_+} f\left(\frac{M}{\omega}\varphi\left(nh - \frac{\pi}{2M}\right)\right) \cos\left(M\varphi\left(nh - \frac{\pi}{2M}\right)\right)\varphi'\left(nh - \frac{\pi}{2M}\right) \quad (\text{C.49})$$

where for large positive n

$$\cos\left(M\varphi\left(nh - \frac{\pi}{2M}\right)\right) \approx \cos\left(mnh - \frac{\pi}{2}\right) = \cos\left(n\pi - \frac{\pi}{2}\right) = 0$$

and the error bound is given by Eq. (C.47).

C.3.2 DE Formula For Fourier Integrals

Consider the Fourier transform

$$F(\omega) = \int_0^\infty f(x) e^{i\omega x} dx \quad (\text{C.50})$$

Here $f(x)$ is slowly converging as $x \rightarrow \infty$ and possibly oscillatory, and ω is large and positive parameter. By applying the transformation (C.43), we obtain

$$F(\omega) = \int_{-\infty}^\infty f(M\varphi(t)/\omega) e^{iM\varphi(t)} (M/\omega)\varphi'(t) dt \quad (\text{C.51})$$

Next define

$$E(\omega) = \int_{-\infty}^\infty f(M\varphi(t)/\omega) e^{iM\varphi(t) - iM\hat{\varphi}(t)} (M/\omega)\varphi'(t) dt \quad (\text{C.52})$$

where $\hat{\varphi}(t) = \varphi(t) - t$. Then, $|E(\omega)|$ is very small for large M , and the order is

$$|E(\omega)| = O(e^{-d' M \omega})$$

where d' is a positive constant depending on $f(x)$ (see Refs [67,68]) . We calculate $\tilde{F}(\omega) = F(\omega) - E(\omega)$ instead of $F(\omega)$. Then,

$$\tilde{F}(\omega) = \int_{-\infty}^{\infty} f(M\varphi(t)/\omega) e^{iM\varphi(t)-iM\hat{\varphi}(t)/2} (2iM/\omega) \sin(M\hat{\varphi}(t)/2) \varphi'(t) dt \quad (\text{C.53})$$

Since $\hat{\varphi}(t) \rightarrow 0$ as $t \rightarrow +\infty$ and $\varphi'(t) \rightarrow 0$ as $t \rightarrow -\infty$, $|\sin(M\hat{\varphi}(t)/2)\varphi'(t)|$ converges to zero as rapidly as $t \rightarrow \pm\infty$. Applying the trapezoidal rule with mesh size h we have

$$\tilde{F}(\omega)_h^{(N)} = \frac{2iMh}{\omega} \sum_{n=N_-}^{N_+} f(M\varphi(nh)/\omega) e^{iM\varphi(nh)-iM\hat{\varphi}(nh)/2} \sin(M\hat{\varphi}(nh)/2) \varphi'(nh) \quad (\text{C.54})$$

Setting $Mh = \pi$ we have

$$\tilde{F}(\omega)_h^{(N)} = \frac{2\pi i}{\omega} \sum_{n=N_-}^{N_+} f\left(\frac{M}{\omega} \varphi\left(\frac{\pi n}{M}\right)\right) e^{iM\varphi\left(\frac{\pi n}{M}\right)-i\frac{M}{2}\hat{\varphi}\left(\frac{\pi n}{M}\right)} \sin\left(\frac{M}{2}\hat{\varphi}\left(\frac{\pi n}{M}\right)\right) \varphi'\left(\frac{\pi n}{M}\right) \quad (\text{C.55})$$

$\tilde{F}(\omega)_h^{(N)}$ converges quickly to $F(\omega)$. The error is bounded as

$$|F(\omega) - \tilde{F}(\omega)_h^{(N)}| < c'_0 e^{-c_0/h} + c'_1 e^{-c_1\omega/h} + c'_2 e^{-c_2\omega/h} \quad (\text{C.56})$$

where c_i, c'_i are positive constants depending on $f(x)$ through d' .

Bibliography

- [1] Agostini, R., Fabre, F., Mainfray, G., Petite, G., and Rahman, N.K., Phys. Rev. Lett., (1979), **42**, 1127.
- [2] Mainfray, G., and Manus, C., Rep. Prog. Phys., (1991), **54**, 1333.
- [3] Keldysh, L.V. (1964), Zh. Eksp.Teor. Fiz. **47**, 1945 [Sov.Phys.-JETP **20**, 1307.
- [4] L.D.Landau, E.M.Lifshitz: Quantum Mechanics: Nonrelativistic Theory, 3rd ed (Pergamon, Oxford 1977).
- [5] Mcpherson, A., Gibson, G., Jara, H., Johan, U., Luk, T.S., McIntyre, I.A., Boyer, K., and Rhodes, C.K. (1987), J. Opt. Soc. Am. B **4**, 595.
- [6] Wildenauer, J. (1987), J. Appl. Phys. **62**, 41.
- [7] Ferray, M., L' Huillier, A., Li, X.F., Lompre', L.A., Mainfray, G., and Manus, C. (1988), J. Phys. B **21**, L31
- [8] Shafer, K.J., Yang, B., Dimauro, L.F., and Kulander, K.c. (1993), Phys. Rev. Lett. **70**, 1599.
- [9] Yang, B., Shafer, K.j., Walker, B., Kulander, K.C., Agostini, P., and Dimauro, L.F. (1993), Phys. Rev. Lett. **71**, 3770.
- [10] Paulus, G.G., Nicklich, W., Xu, H., Lambropoulos, P., and Walther, H. (1994), Phys. Rev. Lett. **72**, 2851.
- [11] Paulus, G.G., Nicklich, W., and Walther, H. (1994), Europhys. Lett. **27**, 267.
- [12] Paulus, G.G., Nicklich, W., Zacher, F., Lambropoulos, P., and Walther, H (1996), J. Phys. B **29**, L249.
- [13] Walker, B., Sheehy, B., Kulander, K.C., and Dimauro, L.F. (1996), Phys. Rev. Lett. **77**, 5031.
- [14] Nandor, M.J., Walker, M.A., and Van Woerkom, L.D. (1998). J. Phys. B **31**, 4617.

- [15] Sheehy, B., Lafon, R., Widmer, M., Walker, B., Dimauro, L.F., Agostini, P.A., and Kulander, K.C. (1998), Phys. Rev. A **58**, 3942.
- [16] Nandor, M.J., Walker, M.A., Van Woerkom L.D., and Muller, H.G. (1999), Phys. Rev. A **60**, R1771.
- [17] Muller, H.G. (1999), Phys. Rev. A **60**, 1341.
- [18] Kulander, K.C., Schafer, K.J., and Krause, J.L. (1993), In "Super-Intense Laser-Atom Physics" (B.Piraux, A.L' Hullier and K.Rzazewski, Eds), Vol **316** of Nato Advanced Studies Institute, Series B; Physics. Plenum, NewYork, P.95.
- [19] Corkum, P.B. (1993), Phys. Rev. Lett. **71**, 1994.
- [20] Bucksbaum, P.H., Bashkansky, M., Freeman, R.R., McIlrath, T.J., and Dimauro, L.F. (1986), Phys. Rev. Lett. **56**, 2590.
- [21] Bucksbaum, P.H., Bashkansky, M., and Shumacher, D.W. (1988), Phys. Rev. A **37**, 3615.
- [22] Mohideen, U., Sher, M.H., Tom, H.W.K., Aumiller, G.D., Wood II, O.R., Freeman, R.R., Bokor, J., and Bucksbaum, P.H. (1993), Phys. Rev. Lett. **71**, 509.
- [23] Reiss, H.R. (1996), Phys. Rev. A **54**, R1765.
- [24] Paulus, G.G., Becker, W., Nicklich, W., and Walther, H. (1994), J. Phys. B **27**, L703.
- [25] Faisal, F.H.M. (1973), J. Phys. B **6**, L89.
- [26] Reiss, H.R. (1980), Phys. Rev. A **22**, 1768.
- [27] Reiss, H.R. (1990), Phys. Rev. A **42**, 1476.
- [28] Reiss, H.R. (1990). In C.A. Nicolaides, C.W. Clark, and M.H. Nayfeh (Eds). "Atoms in Strong Fields", Plenum, NewYork, P.425.
- [29] Reiss, H.R. (1996). In H.G. Muller and M.N. Fedorov (Eds). "Super-Intense Laser-Atom Physics IV". Kluwer, Dordrecht, P.143.
- [30] Lewenstein, M., Balcou, Ph., Ivanov, M.YU., L' Huillier, A., and Corkum, P.B. (1994), Phys. Rev. A **49**, 2117.
- [31] Becker, W., Long, S., and McIver, J.K. (1994), Phys. Rev. A **50**, 1540.
- [32] Becker, W., Lohr, A., and Kleber, M. (1994), J. Phys. B **27**, L325.
- [33] Lewenstein M., Kulander, K.C., Schafer, K.J., and Bucksbaum, P.H. (1995), Phys. Rev. A **51**, 1495.
- [34] Kulander, K.c., Schafer, K.J., and Krause, J.L. (1992). In M.Gavirla (ed). Atoms in Strong Fields., Adv. At. Mol. Opt. Phys. Suppl.1, Accademic, NewYork, P.247.

- [35] Rottke, H., Wolff-Rottke, B., Feldman, D., Welge, K.H., Dör, M., Potvliege, R.M., and Shakeshaft, R. (1994) *Phys. Rev. A* **49**, 4837.
- [36] Cormier, E., and Lambropoulos, P. (1997), *J. Phys. B* **30**, 77.
- [37] Huens, E., Piraux, B., Bugacov, A., and Gajda, M. (1997), *Phys. Rev. A* **55**, 2132.
- [38] Dionissopoulou, S., Mercouris, Th., Lyras, A., and Nicolaidis, C.A. (1997), *Phys. Rev. A* **55**, 4397.
- [39] Ermolaev, A.M., Puzynin, I.V., Selin, A.V., and Vinitzky, S.I. (1999). *Phys. Rev. A* **60**, 4831.
- [40] Glass, D.H., and Burke, P.G. (2000), *J. Phys. B* **33**, 407.
- [41] Cormier, E., Garzella, D., Breger, P., Agostini, P., Chériaux, G., and Lablanc, C. (2001), *J. Phys. B* **34**, L9.
- [42] Volkov, D.M. (1935), *Z. Phys.* **94**, 250.
- [43] Reiss, H.R. (2008), in "Progress in Ultrafast Intense Laser Science" (2008), Springer Series in Chemical Physics **39**, P.1.
- [44] N.B. Delone, and V.P. Krainov "Multiphoton Processes in Atoms" (1994), Springer-Verlag.
- [45] Trombetta, F., Ferrante, G., and Basile, S. (1988), *J. Phys. B* **21**, L539.
- [46] Basile, S., Trombetta, F., Ferrante, G., Barlon, R., and Leone, C. (1988), *Phys. Rev. A* **37**, 1050.
- [47] Jain, M., and Tzoar, N. (1978), *Phys. Rev. A* **18**, 538.
- [48] Mittleman, M.H. (1994), *Phys. Rev. A* **50**, 3249.
- [49] Kamiński, J.Z., Jaroń, A., and Ehlotzky, F. (1996), *Phys. Rev. A* **28**, 1756.
- [50] Kamiński, J.Z., and Ehlotzky, F. (1997), *Phys. Rev. A* **55**, 4625.
- [51] Kamiński, J.Z., and Ehlotzky, F. (1997), *J. Phys. B* **30**, 69.
- [52] Kamiński, J.Z., and Ehlotzky, F. (1997), *J. Phys. B* **30**, 5729.
- [53] Kamiński, J.Z. (1986), *Phys. Scripta* **34**, 770.
- [54] Kamiński, J.Z. (1990), *Phys. Scripta* **42**, 417.
- [55] Kamiński, J.Z. (1988), *Phys. Rev. A* **37**, 622.
- [56] Kamiński, J.Z. (1990), *J. Phys. C* **2**, 7719.
- [57] Milosovic, D.B., and Ehlotzky, F. (1998), *J. Phys. B* **31**, 4149.

- [58] Milosovic, D.B., and Ehloltzky, F. (1998), Phys. Rev. A **57**, 5002.
- [59] Milosovic, D.B., and Ehloltzky, F. (1998), Phys. Rev. A **58**, 3124.
- [60] Eckle, P., Pleiffer, A.N., Cirelli, C., Slaudte, A., Dörner, R., Muller, H.G., Büttiker, M., and Keller, U. (2008), Science **322**, 1525.
- [61] Martiny, C.P.J., Abu-Samha, M., and Masden, L.B. (2009), J. Phys. B **42**, 1.
- [62] Lohr, A., Kleber, M., Kopold, R., and Becker, W. (1997), Phys. Rev. A **55**, R4003.
- [63] Bao, D., Chen, S.G., and Liu, J. (1996), Appl. Phys. B **62**, 313.
- [64] Usachenko, V.I., Pazdzersky, V.A., and McIver, J.K. (2004), Phys. Rev. A **69**, 013406.
- [65] Deng, Z., and Eberly, J.H. (1985), J. Opt. Soc. Am. **2**, 486.
- [66] M.V. Fedorov. Atomic and Free Electrons in a Strong Light Field. (World Scientific, Singapore, 1997).
- [67] Oura, T., Mori, M. (1998), J. Comp. And. Appl. Math. **112**, 229
- [68] Oura, T. (2005), Publ. RIMS., Kyoto Univ., **41**, P.971.
- [69] Leonard I. Schiff. Quantum Mechanics. 3rd edition (Mcgraw-Hill, 1968).
- [70] Henneberger, W., C. (1968), Phys. Rev. Lett., **21**, 838.
- [71] Milton Abramowitz, and Irene I. Stegun, Eds. (1972), Handbook Of Mathematical Functions with formulas, Graphs, And Mathematical Tables., New York, Dover Publications.
- [72] Nordsieck, A., (1954), Phys. Rev. **93**, 785.
- [73] Moshhammer, R., Ullrich, J., Feuerstein, B., Fisher, D., Dorn, A., Schröter, C.D., Crespo Lopes-Urrutia, J.r., Hoehr, C., and Sander, W. (2003), Phys. Rev. Lett., **91**, 113002.
- [74] Rudenko, A., Zrost, K., Schröter, C.D., de Jesus, V.L.B., Feuerstein, B., Moshhammer, R., and Ullrich, J. (2004), J. Phys. B **37**, L407
- [75] Mahrajan, C.M., Alnaser, A.S., Litvinyuk, I., Ranitovic, P., and Cocke, C.L. (2006), J. Phys. B **39**, 1955.
- [76] Chen, Z., Morishita, T., Le, A., Wickenhauser, M., Tong, X.M., and Lin, C.D. (2006), Phys. Rev. A **74**, 053405.
- [77] Gou, L., Chen, J., Liu, J., and Gu, Y.Q. (2008), Phys. Rev. A **77**, 033413.
- [78] Blaga, C.I., Catoire, F., Colosimo, P., Paulus, G.G., Muller, H.G., Agostini, P., and Dimauro, L.F. (2009), Nature. Phys. **5**, 335.

- [79] Quan, W., Lin, Z., Wu, M., Kang, H., Liu, H., Liu, X., Chen, J., Liu, J., He, X.T., Chen, S.G., Xiong, H., Guo, L., Xu, H., Fu, Y., Cheng, Y., and Xu, Z.Z. (2009), Phys. Rev. Lett. **103**, 093001.
- [80] Yan, T., Popruzhenko, S.V., Vrakking, M.J.J., and Bauer, D. (2010), Phys. Rev. Lett. **105**, 53002.
- [81] Dimitriou, K.I., Arbo, D.G., Yoshida, S., Persson, E., and Burgdorfer, J. (2004), Phys. Rev. A **70**, R 061401.
- [82] Smeenk, C., Arissian, L., Zhou, B., Mysrowicz, A., Villeneuve, D.M., Staudte, A., and Corkum, P.B. to be published (private communication)
- [83] Salamin, Y. (1997), Phys. Rev. A **56**, 4910.
- [84] Kopold, R., Becker, W., Kleber, M., and Paulus, G.G. (2001), J. Phys. B **35**, 217.
- [85] Oh, S.D., and Macek, J.H., (1978), Phys. Rev. A **17**, 873.
- [86] Philip J. Davis, and Philip Rabinowitz. Numerical Integration. (Baldsell Publishing Company, 1967).
- [87] Nicholas J. Giordano, and Hisao Nakanishi. Computational Physics 2nd ed., (Pearson Prentice Hall, 1997;2006).
- [88] Tao Pang. An Introduction to Computational Physics. (Cambridge university press 1997).
- [89] J. Mathews and R. L. Walker, Mathematical Methods of Physics, Benjamin, New York (1970).

VITA AUCTORIS

Atef Suleiman Titi was born in the ancient Biblical city of Hebron, in the Holy Land. He was raised in Kuwait. He attended Kuwait University, University of Tennessee, and now at University of Windsor. He is expected to earn his Ph.d in physics in May 2011.