Chapter 1

Introduction

1.1 Motivation and aims

The rapid progress of digital electronics and information technology over the last 40 years has changed the nature and shape of modern society more than any other scientific achievement that has been transferred into the technology. This progress has resulted from the microelectronics industry’s ability to decrease the minimum feature sizes it uses to fabricate the integrated circuits. The most significant benefit for society is the decreasing cost per function, which has led to significant improvements in productivity and quality of life through proliferation of computers, electronic communication and consumer electronics.

One of the technologies behind the phenomenal growth of digital electronics is plasma processing technology. The technology assisted by low-temperature plasma for surface modification processes on a scale of size ranging from nanometers to meters is usually referred to as plasma processing (Makabe and Petrović, 2006). These plasma-based surface modification processes include the plasma enhanced vapor deposition, etching, sputtering, ashing and cleaning. This technology is indispensable for manufacturing the ultra large scale integrated circuits (ULSIs) in microelectronics industry. To maintain the historical trend of reducing the cost/function ratio of integrated circuits, the plasma processing industry must continuously enhance equipment productivity, increase manufacturing yields and most important, increase the number of chips available on a wafer. To this end, a detailed knowledge of the physical and chemical mechanisms within the plasma discharges is required.

Low temperature, weakly ionized or non-equilibrium plasmas are produced by the collisional ionization of the free electrons in a neutral gas under an external electrical power; hence their name of electrical gas discharges. In general, a distinction is made between discharges where all particles (electrons, ions, neutrals) have locally identical temperatures, which is defined as local thermal equilibrium, and the plasmas where the temperatures of the light electrons and of the heavy particles (ions and neutrals) exhibit markedly large differences. In the latter case, the plasmas are said to be in the non-local thermal equilibrium and upon these plasmas we focus our attention in this thesis. The non-equilibrium plasmas could be maintained between metallic or
dielectric electrodes or even in an electrodeless reactor by using electrical power sources ranging from direct current (dc) to radio frequency (rf) energy at frequencies of 50 Hz to 3 GHz. One of the current trends is based on using the plasma sources driven by very high frequencies (VHF: 30 MHz-300 MHz) and also by ultra high frequencies (UHF: 300 MHz-3 GHz) usually with the aid of an external magnetic field. These low temperature plasmas provide a source of ions and radicals responsible for surface modification processes in plasma processing technology.

Plasma discharges are traditionally divided and classified into two regions: the collision-dominated bulk plasma and the sheath (Makabe and Maeshige, 2002). The sheath region surrounds the electrodes or substrates and is characterized by a large spatially inhomogeneous electric field and electrical positiveness. On the other hand, the bulk region is collision dominated and electrically quasi-neutral. The electrons in the bulk plasma play the most important role in both the heating and maintaining of a discharge through the absorbing the power from the external fields and producing the reactive particles (ions and radicals) through the electron-neutral reactive collisions. The highly applied nature of the field has caused a great effort to model both the collision-dominated bulk and sheath plasma regions.

In a collision-dominated regime, two different methods are used to investigate the charged particle kinetics based on a database of molecular collision/reaction processes in gas and surface phases. One method is the fluid model while the other is the particle method (Monte Carlo and particle in cell (PIC)). In the fluid approach, the various plasma species including electrons, ions, radicals and excited neutrals are represented by macroscopic quantities such as particle number density, momentum and energy. The space and time variations of these quantities are described by fluid equations which are derived from the velocity moments of the Boltzmann equation. Surface processes are accounted for in the boundary conditions of the fluid equations. These fluid equations are usually coupled to macroscopic Maxwell equations and through Poisson’s equation the effects of space charge on the electric field distribution is described. In this way, a complete, self-consistent model of a plasma discharge may be obtained. However, among these fluid models there are many implicit and explicit approximations. Usually the fluid equations and associated boundary conditions incorporate restrictive assumptions concerning the charged particle transport. In general however, an accurate description of charged particle kinetics requires a full kinetic treatment, particularly when considering the active plasma components such as electrons and ions.

An alternative approach to the fluid model is the particle approach. In particle models, also known as Monte Carlo models, the individual path of charged particles are followed, where the occurrence and effects of collisions are treated by random numbers. To self-consistently calculate the electric field, particle plasma models require a rather complicated technique, called the particle-in-cell (PIC) technique. Initially, this technique has been primarily developed for a collisionless plasma under a Maxwellian velocity distribution of electrons/ions but later has found its way into the modeling of a collision-dominated plasma discharge. Since Monte Carlo method is infeasible to calculate the paths of all particles, only a number - sufficiently large to produce reliable and smooth results - of representative test particles is followed. From the
test particle paths, macroscopic quantities (density, flux, mean energy), as well as the particle energy distribution function, can be inferred. The biggest advantage of the PIC/MC technique over the fluid approach is the fact that these models can be applied over a wide range of simulation conditions. In practice, however, they need a large computational effort and/or a large computational time. As a consequence, the applicability of this technique in complex discharge geometries and chemistries is of limited use.

The fluid and particle models can be combined in one single model - a hybrid model. In the hybrid models, the Monte Carlo method is used to follow the high energy electrons and map their spatial distribution of ionization. The remaining low-energy particles are described by fluid equations. The hybrid models have a great potential to provide a significant improvement over pure fluid models in the sense that they provide the possibility of adding the full kinetic treatment of electron and heavy particles kinetics (Robson et al., 2005).

The aim of these plasma models is to provide a complete, self-consistent description throughout the entire discharge at the relatively low computational costs. However, this is not an easy task. A complete numerical model of plasma discharges requires the self-consistent solutions of the transport equations for charged and neutral particles, gas-phase and gas-surface interface kinetics and chemistry. At this stage such a model has not been developed and research has been centered on the investigation of specific aspects of the plasma discharge. One of the major aspects in development of these models is a simple but realistic description of charged particle kinetics.

In this work we do not attempt to analyze the complex plasma phenomena in various inhomogeneous plasma regions nor do we attempt to study the space charge effects through a coupling of electron and ion transport properties using Poisson’s equation. Instead we isolate and investigate the electron active component of non-equilibrium plasmas under the action of spatially uniform dc and ac electric and magnetic fields. In particular, in many modeling efforts of the collision-dominated bulk region of non-equilibrium plasmas the description of electron kinetics has turned out to be most difficult and computationally time-consuming part. In general, electrons play the most important role in both maintenance of a discharge, via electron impact ionization and other related processes. Electrons also dissociate the feedstock gas and create the neutral radicals. The knowledge of the distribution function, the ionization and dissociation rates and other transport properties in both space and time is essential to quantify the flow and reaction rates of the plasma kinetics and in particular to determine the fluxes of neutral radicals and ions to the substrate. The modeling of plasmas proceeds through implementation of either transport data or the cross sections for electron-neutral interaction, but in all cases the calculation procedure of the transport properties is a critical step in modeling. This is the main avenue we explore in this work.

In the collision-dominated bulk region of plasma, far away from the influence of the electrodes and physical boundaries, the fields are approximately spatially homogeneous and thus one may consider the boundary free problem often referred to as the swarm problem. A swarm of charged particles is defined to be a collection of such particles of such low density that both the mutual
interactions and the influence of the swarm on the neutral gas distribution can be neglected. The charged particles gain energy from the external fields, and lose energy through binary collisions with the neutral molecules. In the language of plasma physics, this is the so-called free-diffusion limit (White, 1996). If the balance between the energy gain from the external fields and the energy losses in collisions is established, then the transport properties of a swarm can be characterized with space and time independent transport coefficients. In such a case, the hydrodynamic regime prevails. In case of electron swarms, due to the energy input by the electric field, however, the electrons are never in thermal equilibrium with the neutrals and depending upon the interactions, the field strength and the neutral number density, the swarm distributions can vary substantially from the thermal Maxwellian. Moreover, the Coulomb interactions between electrons are to inefficient to restore a Maxwell distribution due to the low degree of ionization of low temperature plasmas. These facts make a kinetic description of the electron component inevitable if an accurate description of the electron heating and transport as well as of the ionization and excitation mechanisms is required.

In plasma modeling community, the hydrodynamic regime is known as the equilibrium state. Of most interest under these equilibrium conditions for plasma modelers are the first few transport coefficients, which include the reaction rate, the drift velocity and diffusion tensor. These transport quantities are necessary input data of fluid plasma models and can both be measured in swarm experiments and determined theoretically through the Boltzmann equation or Monte Carlo simulation.

However, in both plasma discharges and swarm experiments the hydrodynamic conditions are not always satisfied. For instance, in the close vicinity of sources of the primary electrons, the transport properties of the electrons are space dependent. An equilibrium state can be achieved in regions sufficiently far from the source. Typical example of such non-hydrodynamic behavior of the electrons can be found in the steady-state Townsend experiment. Another example is the runaway electrons. This non-hydrodynamic phenomenon is a consequence of decreasing probabilities of electron interactions with neutral particles for electron energies in the range from 100 eV up to 1 MeV (Bakhov et al., 2000). In high electric fields, the electrons gain more energy than they can lose in collisions and hence no steady-state can be reached. This phenomenon was observed in a variety of laboratory experiments and nature and has been the subject of detailed kinetic studies. Finally, the last example of non-hydrodynamic behavior of the electrons is associated with the electron transport in non-uniform fields. If fields changes in space and/or time are too fast to enable relaxation of the charged particles, the non-hydrodynamic behavior develops. The cathode region of a glow discharge or sheath of a rf discharge fall into this category. The electric field varies rapidly with the distance in these regions and so the equilibrium state cannot be reached. Hence the hydrodynamic values of the electron transport properties including Townsend’s first ionization coefficient which is the most important to study the development of a breakdown, should not be used in the analysis of this region.

There are two main methods to study the kinetics of charged particle swarms in neutral gases under both the hydrodynamic and non-hydrodynamic conditions: kinetic Boltzmann equation
and Monte Carlo simulation. Both of these techniques are discussed in this thesis. Aside from the modeling of plasma discharges, it must be emphasized that the nature of the present technique for solving the Boltzmann equation and the concept of a Monte Carlo simulation code developed in this thesis permit their applications to a wide range of physical situations where swarm conditions prevail. Some illustrative examples of these applications include:

- Design and modeling of swarm experiments for the determination of low-energy electron (ion)-molecule cross sections (potentials);
- Design and modeling of the drift chambers for detection particles in high energy accelerators;
- Design and modeling of plasma light sources, plasma displays and gas lasers;
- Development of techniques for detection and removal of atmospheric gas pollutants;
- Development of reactors for surface treatment of polymers, textile and even organic matter.

We believe much remains to be said about the kinetic theory of charged particle swarms in neutral gases. Kinetic modeling of plasma discharges in association with the swarm physics should be the basis in many respects for understanding complex plasma phenomena, breakdown and sustaining mechanisms. In addition, the kinetic modeling of plasma discharges provide the input data for both fluid and hybrid models. However, the recent years have witnessed that the modeling of low-temperature plasmas, and in particular, the description of electron kinetics is going more toward empirical procedures that often oversimplify the process which result in neglecting of some of the well established kinetic phenomena which are particularly abound in electron transport. As an illustrative example, the previous solutions of the Boltzmann equation in modeling the rf plasma discharges involve assumptions, treatments and approximations which limit the range of electric and magnetic field strengths, field frequencies and types of neutral gases. The aim of this thesis is to provide a general kinetic theory and associated computer codes which remove these restrictions. Finally, there is also the intrinsically interesting motivation for the studies of charged particle kinetics in neutral gases under the action of electric and magnetic fields from the pure physics and numerical point of views.

1.2 Nature of the problem and theoretical methods employed

The physical object of our study is a swarm of charged particles moving under the influence of electric and magnetic fields through a spatially homogeneous background of neutral molecules, characterized by a Maxwellian velocity distribution and a Boltzmann distribution of internal states. The number density of the swarm is assumed to be so low that both the charged particle-charged particle interactions and the influence of the swarm on the background molecule gas can be neglected. The behavior of the charged-particle swarms is therefore determined solely through binary collisions with neutral molecules and by the forces exerted by applied electric
and magnetic fields. The collision times between the charged particles of the swarm and neutral molecules are assumed to be negligible in comparison with mean free times. As a consequence, all quantum-mechanical effects can be ignored and the motion of a swarm of charged-particles between collisions can be described with the laws of classical physics. In this thesis we consider elastic, inelastic and non-conservative collisions between the charged and neutral particles.

A swarm of charged particles in neutral gases under the influence of spatially homogeneous and time-dependent electric and magnetic fields crossed at arbitrary angle is described by the Boltzmann equation (Boltzmann, 1872):

\[
\frac{\partial f}{\partial t} + c \cdot \frac{\partial f}{\partial r} + \frac{q}{m} \left[ E + c \times B \right] \cdot \frac{\partial f}{\partial c} = -J(f, f_o);
\]

(1.1)

where \( f(r, c, t) \) is the phase-space distribution function, \( r \) and \( c \) denote the position and velocity coordinates while \( q \) and \( m \) are the charge and mass of the swarm particle and \( t \) is the time. The right-hand side of (1.1), \( J(f, f_o) \), denotes the linear charged particle-neutral molecule collision operator, accounting for elastic, inelastic, and non-conservative (e.g. ionizing or attaching) collisions. The details of this linear integral operator are given in Chapter 4, but we note here that the original Boltzmann collision operator (Boltzmann 1872) and its semi-classical generalization (Wang Chang et al., 1964) are used for elastic and inelastic collisions respectively. The ionization and attachment collision operators employed in this thesis are discussed by (Robson and Ness, 1986).

The theoretical foundations for the solution of the Boltzmann equation in the hydrodynamic regime under the influence of dc electric and magnetic fields crossed at arbitrary angle when non-conservative collisions are operative were formulated by Ness (1993). The numerical solution of the hierarchy of kinetic equations derived by Ness (1993) has been applied to a range of model and real gases for perpendicular electric and magnetic fields (Ness, 1994; Ness and Makabe, 2000). The numerical solution of the conservative Boltzmann equation has been extended to arbitrary angles by White et al. (1999a) and applied for modeling a magnetron discharge in oxygen (White et al., 2005). In this thesis we generalize the previous treatments to include time-dependent electric and magnetic fields crossed at arbitrary angle and non-conservative collisions. We highlight the modifications of the hydrodynamic theory arising from this generalization and apply our theory and associated numerical code to study the electron kinetics in dc and/or rf electric and magnetic fields. The effect of the angles between the fields when non-conservative collisions are operative is investigated for electron swarms in model and real gases. Under such conditions, the most frequently employed approximations in solving the Boltzmann equations are investigated. The validity of the two-term approximation for solving the Boltzmann equation is examined while the inadequacies associated with the expansion of the velocity distribution function in terms of Legendre polynomials and effective field approximations are illustrated and highlighted.

Apart from the theory for solving the Boltzmann equation, in this thesis we present our Monte Carlo simulation code. The initial version of the code developed at the Institute of Physics in Belgrade is improved by introducing new elements. A comprehensive review of the initial version of the code has been recently published (Petrović et al., 2002; Dujko et al., 2005).
Among these new elements, the treatment of the electron swarm motion under the influence of electric and magnetic fields crossed at arbitrary angle is the most significant. The inclusion of an arbitrarily oriented magnetic field with respect to the electric field vector introduces some additional complexity in the electron motion. In such a case, the application of Boris rotation algorithm (Birdsall and Langdon, 1974) widely used for numerical integration of the equation of electron movement for an orthogonal field configuration may not be of much use and has to be replaced by an analytical solution. The code is further improved to follow and sample the spatially resolved characteristics of a swarm of charged particles.

Various important aspects of the electron transport in neutral gases under the action of spatially homogeneous dc electric and magnetic fields are studied in this thesis. Under steady-state dc conditions, we focus on the way in which the transport coefficients and other transport parameters are influenced by the synergism of magnetic fields and non-conservative collisions. In addition, the sensitivity of electron transport coefficients with respect to the energy dependence of the cross section is studied. Another important aspect of the investigation presented in this thesis is the temporal relaxation of electron swarms. In order to analyze the relaxation process and to find its characteristics parameters, like the relevant relaxation time, a consequent kinetic study of the temporal transient processes of the electrons is carried out using appropriate relaxation models. The last segment of the work within the framework of the hydrodynamic studies centers the electron transport properties of a swarm of charged particles in gases under the influence of spatially uniform time dependent electric and magnetic fields. We focus on the way in which the transport coefficients and other transport parameters are influenced by the field frequency, time-resolved magnetic field, phase difference between the fields and angle between the fields.

The second part of the thesis deals with the transport properties of the electron swarms under the action of dc electric and magnetic fields crossed at arbitrary angle in an idealized steady-state Townsend (SST) experiment. As pointed out recently by Li et al. (2006), the application of hydrodynamic theory to study an idealized SST experiment is entirely inappropriate due to the presence of sources of charged particles. The first important step towards modern non-hydrodynamic kinetic studies on charged particle swarm transport in an idealized SST experiment was carried out by Robson et al. (2000). The formal kinetic theory has been presented and it has been shown that the famous Franck-Hertz experiment could be linked to an idealized SST experiment. More details about this issue will be addressed in later chapters. In 2002, the same problem was attacked by Li et al. (2002) and an extension to the earlier non-hydrodynamic kinetic theory has been developed. They developed a formalism for both ions and electrons and consider the situations where both conservative and non-conservative collisions may take place. Finally, in 2006 Li et al. (2006) extended their earlier non-hydrodynamic theory to include a magnetic field at right angles with the electric field and to develop a formalism suitable for dealing with both ions and electrons when only conservative collisions are operative. It should be highlighted that there was an error in reference Li et al. (2002) surrounding numerical application of the boundary at infinity. One of the principal aims of this thesis is to remove these errors and misunderstandings which have plagued the studies on the spatial relaxation
processes of electrons in an idealized SST experiment. The further extension of the previous non-hydrodynamic theory to include the arbitrary configuration of the electric and magnetic field is given in this thesis.

To this end, a comprehensive non-hydrodynamic theory based on a multi-term theory for solving the Boltzmann equation and fully kinetic SST Monte Carlo simulation code have been developed in this thesis. These two techniques are applied to model and interpret the spatial relaxation processes of electrons in an idealized SST experiment. The conservative Boltzmann equation is solved using a “two-temperature” moment method, involving a multi-term Burnett function representation of the velocity distribution function. Numerical calculations are performed and the effects of magnetic field on spatial relaxation characteristics of transport properties are demonstrated. In the context of Monte Carlo studies, a non-trivial extension of the Monte Carlo code to consider the spatial relaxation of the electron swarm under the influence of electric and magnetic fields crossed at arbitrary angle confined to steady-state conditions in infinite plane-parallel geometry is developed. The explicit effects of ionization and attachment on the spatial relaxation profiles are considered using physical arguments. We identify the relations for the conversion of hydrodynamic transport properties to those found in the steady-state Townsend (SST) experiment. Our Monte Carlo simulation code and sampling techniques appropriate to these experiments has provided us with a way to test these conversion formulae and their convergence.

In what follows, some significant factors and particularly turning points in historical development of the kinetic theory of charged particle swarms are outlined. The primary aim is to place theoretical methods developed and employed in this thesis in a historical perspective and to highlight the significance of our research for further advances in modern kinetic theory. In addition, the most interesting hydrodynamic and non-hydrodynamic kinetic phenomena observed in charged particle transport are reviewed with principal aim of highlighting their importance in modeling of low-temperature plasmas and in fundamental kinetic theory.

1.3 Some factors in the historical development of the Boltzmann equation analysis under hydrodynamic conditions

1.3.1 Swarms in neutral gases under the influence of dc electric field

The Boltzmann equation is associated with the famous Austrian physicist Ludwig Eduard Boltzmann (1844-1906). Although the original Boltzmann equation was developed to describe the dynamics of an ideal gas assuming elastic collisions only (Boltzmann, 1872), the form of this equation has not changed since its inception. However, the solution of the Boltzmann equation has undergone extensive investigation especially in the last several decades. From the pure physics point of view, the Boltzmann equation has been ordinarily used as a basic equation to analyze experimental results of all swarm experiments. On the other hand, the investigation towards an accurate solution of the Boltzmann equation was driven by the need for accurate
transport coefficients and transport properties in gases and gas mixtures used for numerous applications ranging from the plasma processing technology, to the wire chambers used in high energy particle detectors and to gas lasers. Both experimental and theoretical work on electron swarms under the action of electric and magnetic fields prior to 1980 is summarized in the book by Huxley and Crompton (1974) and the review article of Heylen (1980). More recent review on historical development of the kinetic theory of charged particle swarms moving in neutral gases under the influence of electric fields is presented by Robson and Ness (1986), White et al. (2002) and Robson (2006).

At the heart of this thesis is the Boltzmann equation for charged particle transport in neutral gases under the influence of time-dependent electric and magnetic fields when non-conservative collisions are operative. Numerous publications devoted to theoretical methods and numerical techniques for solving the Boltzmann equation for charged particle swarms under the influence of electric field only have been reviewed in theses of Ness (1985), Petrović (1985) and White (1996). For the sake of completeness, the most important moments in historical development of the Boltzmann equation will be outlined again but the primary goal of this section is to describe the progress achieved over the last quarter of the last century.

The theoretical methods developed for solving the Boltzmann equation can be generally classified into two distinctively different groups: expansion and integral methods (Li, 1999). In an integral method the Boltzmann equation is solved by direct integration while in an expansion method the distribution function is ordinarily expanded in terms of a series of functions and subsequently solved. Perhaps the best-known and first rigorous expansion method for solving the Boltzmann equation is the Chapman-Enskog method described in great detail by Chapman and Cowling (1939). This method assumes an expansion about the absolute equilibrium solution, a Maxwellian at the neutral gas temperature. This approach is thus valid only for conditions near thermal equilibrium. However, it is well-known that even for moderate electric field strength the electron distribution function can substantially deviate from the Maxwellian (Mason and McDaniel, 1988) and hence in the context of the present problem, the Chapman-Enskog method is not of much use. It should be noted, however, that hydrodynamic expansion used in this thesis is similar to the Chapman-Enskog method, except that the expansion is about the steady-state spatially uniform velocity distribution function rather than the thermal equilibrium one, and hence it is suitable for arbitrary electric field strengths.

A brief survey of literature associated with the kinetic theory of charged particle transport in neutral gases reveals that the theory for electrons has been developed some faster and along a different path in comparison to ion transport theory. Another thing that strikes the reader surveying the literature on kinetic theory of charged particle transport is that the literature is almost strictly divided among the electron and ion transport theory. A classical example is the historical book of Huxley and Crompton (1974) on electron transport in neutral gases and book of Mason and McDaniel (1988) on ions. A glaring exception of this practice is the work of the group at the James Cook University which has developed a detailed unified multi-term theory of electron and ion swarms in dc and even in ac electric fields (White, 2001). The reason
for the more rapid theoretical progress of electron transport theory lies in the large difference
in the ratio of the charge carrier mass $m$ to the neutral gas molecule $m_0$. The small mass
ratio for electrons allows to express the conservative collision integrals in a differential - finite
difference form. Another considerable simplification lies with the fact that in many cases of
interest the distribution function is adequately represented by the first two-terms in spherical
harmonics expansion of the angular dependence in velocity space. This is the well-known two-
term approximation or Lorentz approximation (Lorentz, 1905). In his work on the conduction of
electrons in metals, Lorentz considered anisotropies in the velocity distribution under the action
of the electric field. Further simplifications are also possible. For example, in the presence of
elastic collisions only and under spatially homogeneous conditions the Boltzmann equation can
be solved analytically using the two-term approximation. This was the program carried out by
Pidduck (1916; 1936), Druyvesteyn (1930; 1934), Davydov (1935) and Morse et al. (1935). Note
however, that in the presence of inelastic collisions where the collision operator is expressible
in a finite-difference form (Frost and Phelps, 1962), the analytical solution is generally not
obtainable (White, 1996). In any case, ever since from the early 1900s and Lorentz time, the
two-term approximation has been extensively employed and continues to play important role in
swarm and plasma modeling communities.

However, as pointed out by Robson and Ness (1986) and White et al. (2003) the two-term
approximation is invalid if the distribution function departs substantially from spherical symme-
try in velocity space. Anisotropy of the distribution function is induced when inelastic collisions
play an important role in the energy loss processes. In such a case, the multi-term solution
of the Boltzmann equation must be used. Much efforts have been done in the last 40 years
towards obtaining multi-term solutions of the Boltzmann equation. The first limited extension
for steady state and spatially homogeneous conditions beyond the two-term approximation to
three terms was investigated by Wilhem and Winkler (1969), Ferrari (1975; 1977), Braglia et
al. (1977) and Makabe and Mori (1980) while the extension to four terms has been considered
by Cavalleri (1981) and Braglia et al. (1984). The first accurate systematic multi-term theory
for solving the Boltzmann equation, valid for arbitrary conservative collisional processes and
electric fields was developed by Lin et al. (1979a). In the study of electron swarms this theory
has become known as the moment method, or LRM (Lin-Robson-Mason) theory. The basis of
the LRM theory were the previous ideas for electrons and ions developed by Robson and Kumar
(1971) and previous theory of Viehland and Mason (1975; 1978) for ions. The LRM theory was
extended by Robson and Ness (1986) and Ness and Robson (1986; 1989) to produce the most
accurate multi-term treatment of non-conservative charged particle transport in neutral gases
under the action of electric field.

Within the framework of the present work, the LRM theory and works of Robson and Ness
(1986), Ness and Robson (1986; 1989), Ness (1993; 1994) and White et. al. (1999a; 2002) are
particularly important. This theory utilizes the mathematical machinery developed by Kumar
(1966a; 1966b; 1967) in reformulating the Chapman-Enskog solution using irreducible tensors
and methods traditionally employed in quantum mechanics and nuclear physics. A central point
in this theory is the hydrodynamic assumption of the distribution function (Kumar et al., 1980).
This procedure assumes the swarm has evolved to the hydrodynamic stage, that is, a stage where the space-time dependence of the distribution function is described by linear functionals of the number density. The extension of the hydrodynamic description to time-dependent situations has been addressed by Lin and Bardsley (1977), Kumar et al. (1980), Kumar (1981), Tagashira and Kondo and co-workers (1987; 1990; 1993; 1994), Standish (1987; 1989), White (1996) and White et. al. (1999b; 2002). It is important to note that transport coefficients are defined only in the hydrodynamic regime. In addition, the hydrodynamic approximation separates the space-time dependence of the phase-space distribution function from the velocity dependence.

As already remarked, the traditional treatment for charged particle swarms in both the electric and magnetic fields involves an expansion of the angular part of the velocity dependence in terms of spherical harmonics. The expansion coefficients of the spherical-harmonic expansion of the hydrodynamic components of the distribution function are generally functions of speed (and time in time-dependent situations). In particular, it has been shown by Richley (1999) that instead of expanding the distribution function in spherical harmonics, an ellipsoid of revolution can be used to represent the phase-space distribution function at any point of phase space. Analogous to the two-term spherical harmonic expansion, this ellipsoid can be described by two parameters (one scalar and one vector) that are functions of position, and the magnitude of velocity. This approach was tested against some well-established techniques including the Monte Carlo simulation and it was found that it can be used for nearly isotropic cases (Pinhao et al., 2004). In contrast to the angular dependence of the phase-space distribution function in velocity space, many options are available for the treatment of the speed-dependence including finite-differencing schemes, polynomial expansions, pseudo-spectral methods etc. Some of these methods are detailed in Robson and Ness (1986) and Mason and McDaniel (1988). In traditional kinetic theory, the expansion is made in terms of Sonine polynomials about a variety of Maxwellian-based weighting functions. The combination of spherical harmonics and Sonine polynomials are the well known Burnett functions (Burnett (1935a; 1935b); Chapman and Cowling (1939)), used extensively in kinetic theory in both ion and electron swarms. The utility of a Burnett function basis set lie with the fact these polynomials are orthogonal with respect to any scalar function of speed (including a Maxwellian weight function) and are eigenfunctions of the collision operator for the Maxwell model of interactions (Chapman and Cowling, 1939). Other basis set are available as well; for example, Grad (1949a; 1949b) introduced tensorial Hermite polynomials and used them in his well-known thirteen-moment method for his kinetic theory on rarefied gases. These polynomials are equivalent to each other as shown by (Kumar, 1966a) but from the point of irreducibility the Burnett functions are the most economical.

The works of Viehland and Mason (1975; 1978) and Lin and co-workers (1979a; 1979b) revealed that the convergence of the moment equations is rapidly improved if the Maxwellian weight function can be made to resemble the actual swarm distribution function. This involves the application of Maxwellian weight function whose temperature is not restricted to the gas temperature. For electrons, the so-called two-temperature theory is generally sufficient. Within the framework of this theory, the weighting function is a Maxwellian at a temperature which is not equal to the neutral gas temperature and can be used as a flexible parameter to optimize
convergence. For ions however, more flexibility in the weighting function is required and various ‘theories’ have been formulated including the three-temperature method (Mason and McDaniel, 1988), bi- and multi-Maxwellian weighting functions (Ness and Viehland (1990); White et al. (1999a)), drifted Maxwellians (Ness and Robson, 1985) and Gram-Charlier (Viehland, 1994). More on these various methods can be found in theses of Ness (1985) and White (1996).

In what follows we briefly review other techniques for solving the Boltzmann equation under hydrodynamic conditions. A multi-term theory for charged particle swarms under the action of the electric field only which was able to furnish all transport coefficients was developed by Pitchford et al. (1981) and Pitchford and Phelps (1982). A salient feature in their numerical technique is an expansion of the phase-space distribution function in velocity space in terms of the Legendre polynomials while for a treatment of the speed-dependence the cubic B-splines are used rather than Sonine polynomials or a finite-difference method. In a multi-term approach developed by MacMahon (1983), the velocity distribution function is expanded in terms of the Legendre polynomials while a finite-difference method is used to solve a modified Boltzmann equation. In his method, the Boltzmann equation is modified by the addition of a term introduced to ensure convergence of the iterative procedure. As the iteration proceeds the additional term tends to zero and the converged solution is actually the desired solution to the Boltzmann equation. Other iterative methods include the method of Kleban and Davis (1977), path integral methods of Skullerud and Kohn (1983) and Segur et. al. (1983; 1984), the finite element approximation of the Boltzmann equation (Segur et al. (1984) and Yousfi et al. (1985)) and the so-called exact Boltzmann equation analysis of Tagashira et al. (1978) and Kitamori et. al. (1978; 1980). It should be noted that majority of these techniques (except Yousfi et. al. (1985)) are able to deal with the conservative Boltzmann equation only. In 1988 Yachi et al. (1988) developed a multi-term theory in which at first the two-term solution is obtained while the high-order terms are generated subsequently by applying a Galerkin technique. This theory was developed for the pulsed Townsend conditions while in 1991 their multi-term theory was extended to consider the time of flight electron transport parameters when non-conservative collisions are present (Yachi et al., 1991).

One of the main motivating factors behind both the swarm experiments and Boltzmann equation analysis of charged particle transport is the determination of low-energy electron (ion)-molecule cross sections. While the knowledge of low-energy electron (ion)-molecule cross sections is of a fundamental importance from the pure physics point of view, any practical application of these cross sections requires their provisional renormalization to fit the swarm data. This can be done through the so-called inversion procedure where the cross sections are adjusted until some preset agreement is obtained between experimentally measured and theoretically calculated transport coefficients. Perhaps the first use of transport theory to obtain collision cross sections was that of Townsend and by Ramsauer in the early 1920s. These early methods were based on measuring the drift velocity in a gas as a function of $E/p$ (electric field strength divided by a gas pressure), and inverting the integral relating the drift velocity and momentum transfer cross section using an approximate expression for the energy distribution of the electrons. In the 1960s Phelps and many other collaborators developed algorithms for solving the Boltzmann equation
for transport of electrons in gases to obtain the electron transport coefficients and distribution function valid for higher fields and in the presence of inelastic collisions (Phelps, 1968). At the same time, the swarm experiments of the drift velocity and transverse diffusion coefficient in an electric field increased in accuracy and hence it became possible to make comparisons between cross sections obtained by the swarm method and beam experiments. The swarm methods of deriving cross sections developed by Phelps and collaborators became accepted as competitive and complementary to other established techniques, such as crossed-beam or total attenuation experiments, particularly in low energy range where these experimental techniques are faced with a wide range of systematic problems if absolute values of integral cross sections are required. The gas laser modeling community was the first to benefit from very accurate momentum transfer and lower energy inelastic cross sections that have been derived from measurements of the drift and diffusion of electron swarms in gases.

The swarm technique of deriving cross sections has increased in sophistication over the years. The review papers of Crompton (1994) and Petrović et al. (2007) outline the current status in the field. Originally a two-term approximation for solving the Boltzmann equation was used to unfold the transport data, but subsequent multi-term calculations of Haddad and Crompton (1980), Ness and Robson (1986), Yachi et al. (1988) and Yousfi and Benabdessadok (1996) revealed a large discrepancy between the cross sections obtained with these two techniques. In spite of these and many other well-known examples which illustrate the inadequacies of a two-term theory, there are many public domain Boltzmann solvers based on the two-term approximation and specifically developed for the cross section adjustments. The illustrative examples include the ELENDIF (http://www.kinema.com/prod03.htm) developed by Morgan and Penetrante (1990) and BOLSIG (http://www.siglo-kinema.com/bolsig.htm) developed by W.L. Morgan, J.P. Boeuf and L.C. Pitchord. Even the fully automated numerical optimization procedures to manipulate the input cross sections based on a two-term theory have been developed and extensively used for a wide range of gases (Taniguchi (1987); Morgan (1991; 1993). One of the principal aims of this thesis is to sound a warning to those who use these public-domain codes to be aware of the inherent inaccuracies associated with the two-term approximation. Generally speaking, one may never be sure that the two-term approximation hold the necessary accuracy to obtain the realistic cross sections until multi-term theory (or Monte Carlo simulation) has been run as a check.

The Boltzmann equation analysis has played an important role in understanding some of the well-known kinetic phenomena in electron transport. The term ‘kinetic phenomena’ may be used for a class of phenomena associated with behavior of an ensemble of charged particles that may not be trivially predicted on the basis of individual collision events and effect of the fields. It is easy to predict that there will be a lot of phenomena associated with source boundary effects that may be described as non-hydrodynamic but there are plenty of phenomena that occur even in hydrodynamic situations. Perhaps one of the first kinetic phenomena that was explained using a Boltzmann equation analysis was that of anisotropy of the diffusion of the electrons in neutral gases (Parker and Lowke (1969a; 1969)). Such phenomena analyzed on the basis of the Boltzmann equation analysis include:
- Negative differential conductivity (Petrović et al. (1984); Robson (1984)).
- Negative transient mobility (Shizgal and MacMahon, 1985).
- Negative absolute mobility (Dyatko et al. (1998; 1999; 2000; 2001)).

Finally there is a whole range of effects in electron transport induced by: (i) non-conservative collisions (attachment/ionization) (see for example Yoshida et al. (1983); Ness and Robson (1986); Itoh et al. (1991); Nolan et al. (1997)); (ii) vibrationally-excited molecules (Aleksandrov and Kochetov, 1993); (iii) electron-electron collisions (Sa et al. (1992); Yousfi et al. (1992); Dyatko et al. (1993); Dyatko et al. (2003)). Such phenomena are further complicated by the presence of rf fields and can be explained using a Boltzmann equation analysis as well. Some of these kinetic phenomena have been reviewed recently by the groups at the Institute of Physics in Belgrade (Serbia) (Petrović et. al. (2002; 2007)) and James Cook University in Townsville (Australia) (White et al., 2002).

1.3.2 Swarms in neutral gases under the influence of dc electric and magnetic fields

Even the early studies of charged particle transport in neutral gases were concerned with the effects of a magnetic field, mostly because a major motivation was the influence of a magnetic field on ionization and breakdown mechanism. Both theoretical and experimental early work on motion of charged particle swarms in gases under the influence of electric and magnetic fields has been reviewed by Allis (1956), Heylen (1980) and Huxley and Crompton (1974). More recent results with particular emphasis on theoretical and numerical methods for solving the Boltzmann equation for charged particle swarms in electric and magnetic fields have been reviewed by White et al. (2002).

A brief survey of the early literature prior to 1993 associated with techniques for solving the Boltzmann equation for swarms in neutral gases under the influence of electric and magnetic fields reveals the following inadequacies among these techniques: (i) A restriction to two-term truncations in the Legendre polynomial expansion of the velocity dependence (Winkler (1972); Huxley and Crompton (1974)); (ii) Restrictions to limited interaction models (Braglia and Ferrari (1973a; 1973b)) and (iii) Restrictions to spatially-homogeneous swarms and effective field concepts. Biagi extended the two-term formalism of Huxley and Crompton (1974) to three term theory (Biagi (1988; 1989)). The MAGBOLTZ code was developed on the basis of this theory and extensively used in the particle detector community for the determination of electron transport coefficients for arbitrary angles between the electric and magnetic fields. The significant limitations of Biagi’s theory and associated code have been addressed by Ness (1993), Robson et al. (1997) and White et al. (1999a). The major limitation arises from incorrect symmetry assumptions in velocity space. As pointed out by Ness (1993), if the magnetic field is present a two-term Legendre polynomial expansion is strictly valid only for spatially homogeneous swarms for the case of parallel fields. As a consequence of this critique, Biagi has abandoned any further
development of the code based on the Boltzmann equation and later he developed a new code based on a Monte Carlo method (Biagi, 1999).

Perhaps the first theory which avoids the restrictions given above was that of Kelly (1960). He developed a multi-term theory valid for arbitrary angles between the fields following the previous works of Landshoff (1949) and Grad (1949). As noted by White et al. (1999a), many authors failed to acknowledge the work of Kelly although his method for solving the Boltzmann equation was based on a firm theoretical basis. Another example of works which falls into this category is that of Viehland et al. (1975). They applied the two temperature moment method to solve the spatially homogeneous Boltzmann equation for ions in the presence of both electric and magnetic fields. During the 1980s the Monte Carlo method has been extensively used to analyze the effects of a magnetic field on charged particle swarms (see next section). In contrast, comparatively little work has been done on charged particle swarm transport in the presence of both electric and magnetic fields via Boltzmann equation analysis. The lack of systematic approach in solving the Boltzmann equation was perhaps the major reason. However, during the 1980s and at the beginning of 1990s it became evident that any further advances in plasma technologies for integrated circuits, high-energy particle detectors, gas lasers and high-current switches could not be made without detailed understanding of charged particle transport in neutral gases under the action of both electric and magnetic fields. As remarked previously, within the particle detector community Biagi extended the two-term theory of Huxley and Crompton (1974) while Ikuta and Sugai applied the so-called flight integral method (Ikuta and Sugai, 1987) to the Boltzmann equation for a Lorentz swarm in a model gas for both parallel and perpendicular field configurations (Ikuta and Sugai, 1989). It was shown later by Robson (1995) that their definition of diffusion is inconsistent with well established kinetic theory. The numerical calculations of the diffusion coefficients based on a moment method for solving the Boltzmann equation of Ness (1994) were in a strong disagreement with those of Ikuta and Sugai. Subsequent calculations of White et al. (1997) supported the moment method of Ness (1994).

Another source of motivation for studies of charged particle swarms in electric and magnetic fields came from the need to develop and model gas lasers. As an illustrative example, following the previous work of Carleton and Megill (1962), Li and Chen (1993) have considered the effects of a magnetic field on electron transport using the Boltzmann equation for a magnetically confined CO\textsubscript{2} laser. The Boltzmann equation is solved under the spatially-homogeneous conditions and hence the presented transport coefficients as a function of $B/n_0$ are of limited use.

In 1993 Ness presented a general formalism for solving the Boltzmann equation for charged particle swarms in the presence of both the electric and magnetic fields (Ness, 1993). This theory was developed in order to assist with the interpretation of the swarm experiments carried out in a crossed field configuration (Schmidt (1993); Schmidt (1994)). The experiments are made for a simultaneous measurement of drift velocity and diffusion tensor components of electrons in counting gas mixtures. The application of an orthogonal configuration of electric and magnetic fields gives rise to an additional number of transport coefficients and thus one is able to exploit this in the inversion procedure. Thus by varying the magnitude of a magnetic field an additional check on the validity of a cross section set may be made through electron swarm data. This
procedure has been used for a fine adjustment of the momentum transfer cross section in elastic collisions for rare gases (Schmidt, 1994). The multi-term theory of Ness (1993) is based upon the spherical harmonics decomposition of swarm particle velocity distribution function for charged particle swarms in neutral gases under the influence of electric and magnetic fields crossed at arbitrary angle. A salient feature of this theory is that no assumptions are made about the mass of swarm particle and hence it is valid for both the electrons and ions. The result of this work is a set of kinetic equations which can be solved by a wide range of numerical techniques. This was the program of subsequent work of Ness (1994) where the numerical solution has been applied to a range of model and real gases but only for electrons undergoing conservative collisions. In order to optimize the radial resolution of the time projection chambers, the same approach has been employed for studies of electron drift and diffusion in gas mixtures of argon and molecular gases including CO₂, CH₄ and DME (dimethylether \((\text{CH}_3)_2\text{O}\) (Bittl et al., 1997). In 1999, White et al. (1999a) extended the numerical solution of the conservative Boltzmann equation by (i) considering the effects of the angle between the fields on electron transport and (ii) representing the speed dependence of the phase-space distribution function in terms of an expansion in Sonine polynomials about a weighted sum of Maxwellian distributions at different temperatures (the so-called multi-Maxwellian expansion). The effect of the angle between the fields on both transport coefficients and distribution function and the inadequacies of expansions in terms of Legendre polynomials and effective field approximations have been addressed by White et. al. (1999a; 1999c; 1999d; 2001).

The next two papers published by the group at the James Cook University and co-workers are particularly important in the context of plasma modeling. In 2000, Ness and Makabe (2000) extended the numerical solution to include ionization by electron impact, a non-trivial extension of the associated code. They considered the synergism of ionization processes and magnetic field on electron transport in pure argon. As previously remarked, studies of charged particle transport in gases in combined electric and magnetic fields play a crucial role in low temperature plasma processing devices, such as magnetron sputtering devices and ICP (inductively coupled plasma) reactors. There have been numerous studies of magnetron discharges (see for example Shon and Lee (2002) and Nanbu et al. (2000) and references therein) but the recent two-dimensional hybrid model is of particular note (Shidoji et. al. (1999; 2001)). In this hybrid model, the low-energy electrons and ions in the collision-dominated bulk plasma region are treated using a fluid model while the fast, non-equilibrium electrons in the cathode region are treated by a Monte Carlo simulation. The fluid part is based on the local field approximation and requires the tabulation of electron transport coefficients as a function of the reduced fields \(E/n_0\), \(B/n_0\) and the angle between the fields, where \(n_0\) is the neutral number density. The calculated transport coefficients of Ness and Makabe (2000) have been used in modeling of an argon magnetron plasma (Shidoji et al., 2001). The further extension of the numerical solution include the recent work of White et al. (2005) who considered the electron transport coefficients required for the modeling of bulk electron transport in an O₂ magnetron discharge. As remarked previously, modeling of ICP plasma reactors can greatly benefit from the studies of charged particle transport processes in gases in combined electric and magnetic fields. A recently
developed two-dimensional, time-dependent model for the collision-dominated ICP, based on the relaxation continuum (RCT) theory, employs scaled dc electron transport coefficients in electric and magnetic fields (Kamimura et al., 1999). These scaled dc transport data include the drift velocity and diffusion coefficient. For arbitrary field directions, the drift velocity components are derived in terms of drift velocity components for the parallel and orthogonal fields while the diffusion is assumed to be isotropic and estimated from the momentum balance of electrons. Clearly, further advancements of such and similar models are directly dependent on accurate modeling of charged particles transport.

All in all, as remarked by Dujko et al. (2005) the works of Ness (1993; 1994), White et. al. (1999a; 1999c; 1999d; 2001; 2002) and Ness and Makabe (2000) are the most comprehensive, accurate and detailed of all the studies done on electron transport in electric and magnetic fields in the literature. In this thesis a further extension of numerical solution of the Boltzmann equation is done. Within the framework of dc studies presented in this thesis, the effects of ionization and attachment on electron transport for arbitrary fields between the electric and magnetic fields are investigated. We employ a series of model gases including the Reid ramp model (Reid, 1979), the ionization model of Lucas and Saelee (Lucas and Saelee, 1975) and modified attachment model of Ness and Robson (Ness and Robson, 1986). The results obtained by a multi-term theory for solving the Boltzmann equation are compared with those obtained by a Monte Carlo method and hence the most comprehensive benchmark calculations of electron transport in electric and magnetic fields for arbitrary angles in the literature is made.

1.3.3 Temporal relaxation processes of electron swarms in dc electric and magnetic fields

Before we embark on a journey through the many and varied kinetic phenomena in electron transport in ac electric and magnetic fields, in what follows we give a brief introduction into the great importance of electron relaxation processes in neutral gases. In recent years interest in temporal relaxation processes of charged particles in neutral gases has been revived. This interest was motivated by the desire to understand various transient processes of the electrons in low-temperature plasmas. Relaxation processes of a swarm of charged particles are related to various problems of gaseous electronics such as modeling of non-equilibrium plasma discharges, high-speed switching technique, swarm physics and physics of gas lasers (Winkler et al., 2002). The knowledge of temporal relaxation is essential for a better understanding of electron-molecule interaction as well as for a better understanding of transient transport phenomena in gases such as transient negative electron mobility (Warman et al., 1985) or transient negative electron diffusivity (White et al., 2008). In the context of plasma modeling, the relaxation times of the electron transport properties are necessary input data for fluid plasma models such as the relaxation continuum model (Nakano et al., 1994). However, perhaps the most important motivation factors behind the studies of temporal relaxation of charged particle swarms lies with the fact that full understanding of complex temporal profiles of a particular transport coefficient/property in ac fields requires systematic investigation of the temporal relaxation profiles.
of that transport coefficient/property in dc fields.

A long history with respect to various aspects of the temporal relaxation of the electrons can already be found in the literature (Winkler et al., 2002). The temporal relaxation of the electrons under field-free conditions or the so-called electron thermalization in gases is the first aspect which deserves more mentioning. Thermalization of a non-equilibrium distribution of energetic electrons in a moderator of atomic and/or molecular constituents is an important fundamental problem in chemical physics and radiation chemistry with numerous practical applications. A number of methods to treat this problem have been developed, and have been successfully applied to a variety of gases, e.g. the Monte Carlo method (Koura (1983; 1984; 1985; 1986a; 1986b; 1987a; 1987b)), the Boltzmann equation analysis (Yousfi and Chatwiti (1987); Shizgal and co-workers (Shizgal and Hatano (1988); Shizgal and Ness (1987)) and Kowari and co-workers (Kowari et al. (1992); Kowari and Shizgal (1994); Kowari (1996))) or formalism used in radiation chemistry based on the Spencer-Fano equation (Spencer and Fano, 1954). Robson (1976) employed a variational method to solve the Boltzmann equation taking into account both elastic and inelastic electron-molecule collisions in his study on a diffusion cooling of thermal electrons for certain model and real gases. Similar but not identical method was applied by Skullerud (1983) to analyze the effects of attachment cooling in molecular oxygen. In particular, a kinetic approach for the study of the thermalization of electrons due to elastic collisions in the very low energy regime based on the Fokker-Planck equation (FPE) near thermal equilibrium was developed by Shizgal and coworkers (Shizgal and MacMahon (1985); MacMahon and Shizgal (1985); Viehland et al. (1988)). The essence of their approach is the use of the discrete-ordinate method or the so-called pseudo-spectral method based on a Gaussian quadrature rule for numerical integration. For the electron thermalization problem, the collision operator is approximated by the differential Lorentz-Fokker-Planck operator, owing to the small electron-molecule mass ratio. The formalism of this method has been extended and modified by taking into account the loss of electrons (or positrons) by the attachment Ness and Shizgal (1987) (or annihilation processes Shizgal and Ness (1987)). Further improvements of their method include the correct implementation of the inelastic processes in the collision operator with the goal of understanding the thermalization of electrons in molecular gases (Kowari et al., 1992). Considerable contributions in this field have been made also by Mozumder (1980a; 1980b; 1981; 1982), Bronić and Kimura (1995; 1996) and Hatano and co-workers (Shizgal and Hatano (1988); Okigaki et al. (1982)). Mozumber (1980a;1980b) and Tembe and Mozumder (1983; 1984) have studied the zero-field parameters in pure and mixed atomic and molecular gases. Their method is based on the lowest-order Enskog approximation in which the energy distribution function is assumed pseudo-Maxwellian with a time-dependent temperature. Generally speaking, the common thread among these studies was desire to understand the temporal evolution of the electron velocity distribution function (EVDF) when both elastic and inelastic collisions are operative at various gas temperatures. The key quantity behind these studies was thermalization time. The thermalization time literally means a time until electrons thermalize. It should be noted, however, that in practice the term “thermalization time” is used in different contexts. For example, Warman et al. (1975) measured the thermalization time $\tau_{1,1}$ in H$_2$. The thermalization time $\tau_{1,1}$ is a time until the
average energy of electrons reaches 10% above the thermal energy. More recently, Dujko et al. (2008a) have studied the thermalization of positrons in neutral gases with the goal of improving and optimizing the positron traps. Again the key quantity was thermalization time of some positron transport properties.

Comprehensive studies on the temporal relaxation of the electrons in neutral gases in the last years revealed the large variety of the relaxation phenomena under different conditions. This was the program of many groups and in what follows we briefly review the major contributions in the field. In the 1970s and 1980s the temporal relaxation of a swarm of charged particles in neutral gases in an electric field has been studied by means of Monte Carlo method (McIntosh (1974); Braglia (1977); Lin et al. (1977); Braglia and Baiocchi (1978)) and by solving the Boltzmann’s initial value problem (Skullerud (1974); Tagashira et al. (1978), Kitamori et. al. (1978; 1980); Kondo (1987)). Kumar (1984) developed an eigenvalue theory for solving the Boltzmann equation mainly concerning temporal evolution of the distribution function in a finite enclosure. Jiang and Economou (1993) have studied the temporal evolution of the electron energy distribution function (EEDF) and the electron swarm parameters in oxygen and chlorine. In their work, the spatially homogeneous Boltzmann equation is solved for both dc and ac electric fields by a finite-element method. More recently, Sebastian and Wadehra (2005) have solved the spatially homogeneous Boltzmann equation in order to study the temporal relaxation of the electrons in mixtures of argon and methane. However, as already remarked, the works of Shizgal and co-workers attract special attention. Shizgal and collaborators have studied the relaxation behavior of a swarm of charged particles when non-conservative collisions strongly affect the transport properties. It is interesting to note that in their method the expansion of the distribution function in terms of Burnett functions is avoided because the condition concerned is the case where the attachment cross section is too large, the electron distribution function will be localized sharply in the higher-energy region (i.e. attachment heating), and the Burnett basis expansion is poor at obtaining convergence of numerical results. The method employed in his works is based on the two-term approximation of the expansion in Legendre polynomials of the distribution function. The salient feature of their method is the fact that the Boltzmann equation was rewritten using the Fokker-Planck operator, in which the eigenvalue problem can be transformed to a Schrodinger equation giving very rapid convergence of the eigenvalues, with the procedure of a discrete ordinate method (Shizgal and MacMahon (1985); Ness and Shizgal (1987)). In contrast to Shizgal and co-workers, Kondo and Tagashira (1993) and Kondo et. al. (1994) applied the similar but not identical strategy for solving the Boltzmann equation. The Boltzmann’s initial value problem has been discussed formally with respect to swarm experiments and solved numerically using the Fourier transformation technique. Their method is more connected to the traditional kinetic theory since the analytical expressions for the matrix elements have been calculated in the Burnett basis functions using the two-temperature theory developed by Viehland and Mason (1975; 1978) and Lin et. al. (1979a; 1979b). However, instead of full spherical-harmonics representation of the distribution function, the Legendre polynomial expansion procedure was used and hence only the temporal relaxation of the so-called longitudinal transport coefficients has been studied. However, it should be noted that the effects
of non-conservative collisions on the drift velocity are properly accounted for through the distinction between the flux and bulk values. In addition, one ought to mention the Monte Carlo studies of the temporal relaxation of the EEDF and the electron transport parameters for the Reid ramp model (Bzenič (1997); Raspopović (1999)) and for CF$_4$ (Dujko et al., 2005).

The group at the Institute for Low-temperature Plasmas in Greifswald (Germany) has also made significant contributions in the field. Their initial investigations of the temporal relaxation of the electrons in gases are mainly performed by solving the spatially homogeneous Boltzmann equation using a two-term approximation of the expansion in Legendre polynomials. The resultant system of two partial differential equations for the isotropic and anisotropic parts of the velocity distribution function, is simplified by the quasi-steady-state description of the distribution anisotropy. The limitations associated with the quasi-stationary treatment of the anisotropic component of the distribution function have been investigated by Braglia et al. (1995) and Winkler et al. (1995). In order to avoid these limitations and in order to improve the accuracy of their treatment of the electron kinetics, they have developed a multi-term method to solve the spatially homogeneous Boltzmann equation (Loffhagen and Winkler, 1996a). Their program was to investigate the temporal relaxation of the electrons in neon and to test the so-called conventional approach (the two-term approximation in Legendre polynomials with the quasi-stationary treatment of the anisotropic component of the distribution function) and the strict two-term approximation (the two-term approximation in Legendre polynomials with full time-dependence of both expansion coefficients) against multi-term approach. Similar investigation has been carried out for the temporal relaxation of the electrons in helium, xenon and molecular nitrogen (Loffhagen and Winkler, 1996b). The relatively large deviations between the relaxation profiles of various transport properties obtained by two-term approaches and multi-term method were identified, particularly in the initial and intermediate relaxation stages. The same technique for solving the Boltzmann equation was used to investigate the temporal evolution of the EVDF, mean energy and drift velocity in an Ar/F$_2$ mixture under conditions when the electron number density temporally decreases as a result of the electron attachment to fluoride molecules (Dyatko et al., 2001). The multi-term results confirmed predictions on the occurrence of negative electron mobilities in such a decaying Ar/F$_2$ plasma, which were made in a former study using the conventional two-term approximation and Monte Carlo simulation (Dyatko et al., 2000).

The temporal relaxation of the electrons in the presence of both electric and magnetic fields has been investigated by Loffhagen and Winkler (1999). Within the context of theory and application of theory presented in this thesis, the contribution of Loffhagen and Winkler (1999) deserves special mention. They employed a strict two-term approximation of the spherical harmonics expansion of the EVDF for solving the spatially homogeneous Boltzmann equation for the electrons in neon under conditions where dominant energy transfer is realized through the electronic excitation. In their study, the relaxation process starts from the steady-state acted upon by a dc electric field. At time $t = 0$, a magnetic field is switched on while the electric field is left to be unaltered. The temporal profiles of various transport properties are monitored as a function of time. Similar relaxation model is employed in this thesis. However, it is important
to note that the study of Loffhagen and Winkler (1999) is extended in this thesis by: (i) overcoming the inherent inaccuracies of the two-term approximation; (ii) addressing the temporal relaxation of spatial inhomogeneities through a study of the diffusion tensor; and (iii) highlighting the explicit modification of the electron transport coefficients about by non-conservative collisions of electron attachment and ionization. In this thesis, the spatially inhomogeneous time-dependent Boltzmann equation is solved for the electrons under the influence of both the electric and magnetic fields for certain model and real gases when non-conservative collisions are operative. In recently published papers of White et. al. (2006) and Dujko et. al. (2008a; 2008b) the preliminary results were presented. In this thesis, however, we present the first systematic investigation of the temporal relaxation of the diffusion coefficients and other transport properties under conditions when the electron transport is strongly affected by non-conservative collisions.

1.3.4 Swarms in neutral gases under the influence of ac electric field

The biggest source of motivation for early studies of electron transport in gases in time-dependent fields came from the need to understand the interaction of electromagnetic waves with ionosphere (Mimno, 1937) and breakdown mechanisms in gases in rf and microwave fields (Brasefield (1930a; 1930b)). The first theoretical study of the motion of electrons under an alternating electric field using the Boltzmann equation was outlined by Chapman and Cowling (1939). The major players in these early days were Holstein (1946), Margenau and co-workers (Margenau (1946); Margenau and Hartman (1948)), Hartman (1948) and McDonald and Brown (1949a; 1949b). In 1946 Holstein (1946) applied the Legendre polynomial expansion procedure (neglecting all terms except the first two) to solve the spatially homogeneous Boltzmann equation for electrons located between two plane-parallel electrodes in a high frequency electric field. His work accounted for inelastic processes and established the first connection between distribution functions obtained under ac and dc conditions. He observed that the distribution function associated with an ac field of amplitude $E_0$ is, in limit of low field frequency, identical with the distribution function associated with a dc field $E = E_0/\sqrt{2}$. In the analysis of ionosphere problems, it is necessary to know the conductivity of an ionized gas as a function of electron number density, pressure of the gas and frequency of the waves. This was the program of Margenau (1946) who employed a two-term Legendre expansion of the distribution function in velocity space and a first order Fourier expansion truncation in time. By doing so, this theory was restricted to the field frequencies greater than the total energy transfer collision frequency. The subsequent works of Margenau (1946) and Margenau and Hartman (1948) are of special note. Margenau (1946) applied the same combined Legendre-Fourier decomposition of the distribution function for solving the Boltzmann equation when both elastic and inelastic collisions are operative in order to study the electron diffusion. This work represents the first study of the electron diffusion in an alternating electric field. This theory was generalized by Margenau and Hartman (1948) and should be remembered as a first exact treatment of spatially homogeneous electron swarms in ac electric field valid for arbitrary field frequencies and field strengths. The further extensions of the so-called ‘effective field concept’ of Holstein (1946) and Margenau and Hartman (1948) were
developed by Brown, McDonald and co-workers (McDonald and Brown (1949a; 1949b); Allis and Brown (1952); Rose and Brown (1955)) in their investigation of breakdown mechanisms in high frequency gas discharges. The aim of these works was to calculate the breakdown electric fields at high frequencies in gases on the basis of kinetic theory. It was shown that their effective dc field approximation is valid if the total momentum transfer collision frequency is independent of energy and/or is valid in the high frequency regime where the field frequency is much greater than the total energy transfer collision frequency. Due to the fact that the collision frequencies in helium and hydrogen are efficiently constant over the range of electron energies critical for the development of breakdown in these gases, this method was used to calculate the breakdown electric fields. An excellent agreement between experimentally measured and theoretically calculated breakdown electric fields as a function of the field frequencies validates their approach and represents one of the first triumphs of the kinetic theory in the field of gas discharge physics. All in all, in these early investigations it was convincingly shown, that the breakdown phenomena depend crucially on the EDF form, and the solution of the Boltzmann kinetic equation is necessary for their adequate description.

Along similar lines and independently in the review papers of Allis (1956) and Ginzburg and Gurevich (1960) and textbooks of Holt and Haskell (1965) and Huxley and Crompton (1974), the Legendre-Fourier decomposition technique and effective field approximations were generalized for various collisional processes and field configurations. Advancements in numerical methods and computer power during the 1980s have resulted in more detailed extensions to these earlier theories. However, these improved theories still had severe restrictions on the field frequency and gas types. As an illustrative example, the effective dc field theory was extended by Ferreira and Loureiro (1983; 1984; 1989) to account for energy varying collision frequencies by introducing a ‘representative’ momentum transfer collision frequency. As suggested by Ferreira et al. (1991) this quantity can be chosen quite arbitrarily but in general its value should be close to a value that corresponds to representative electrons of the bulk distribution. Another disadvantage associated with this method lies with the fact this technique is restricted to the high frequency and spatially homogeneous atomic discharges only. For molecular gas discharges at frequencies and pressures that are critical for applications in plasma processing technology, the energy distribution function is generally modulated in time and has a phase-lag with respect to the applied electric field and hence the effective field approximation is not satisfactory approach to describe these plasmas. Despite of these limitations, this procedure has been routinely employed in plasma modeling community (Ferreira et al. (1991); Wang et al. (1993); Kortshagen and co-workers (1991; 1992a; 1992b; 1993; 1993; 1996a)).

The first time resolved solutions to the conservative Boltzmann equation in a spatially homogeneous rf plasma were developed by Wilhem and Winkler (1979) and Winkler et. al. (1984a; 1984b; 1985; 1986). They employed a two-term approximation with quasi-stationary treatment of the anisotropic component of the distribution function and non-stationary treatment of the isotropic component. They refer to this as the ‘strict’ non-stationary solution technique. The quasi-stationary treatment of the anisotropic component limits their method to the frequency regime in which the field frequency must be much less than the frequency for momentum dis-
sipation. However, this technique avoids the limitations associated with a finite Fourier-series truncation and has been used to investigate the frequency limits associated with low-order truncation of Fourier-series expansions and effective field approximations (Winkler et. al. (1984a; 1984b)). The ‘strict’ non-stationary technique was also applied in studies of kinetics of excited states in rf plasmas (Capitelli et. al. (1986; 1987; 1988); Winkler et. al. (1987a; 1987b)). The same method has been applied by other groups (Kohler et al. (1991); Karoulina and Lebedev (1988; 1992) and Goedheer and Meijer (1993)). One of the most frequently used public domain codes ELENDIF (Morgan and Penetrante, 1990) in plasma modeling community also assumes a quasi-stationary treatment of the anisotropic component of the distribution function. In association with the discrete ordinate or the so-called pseudo-spectral method of Shizgal and co-workers (Shizgal and MacMahon (1985); MacMahon and Shizgal (1985)), a quasi-stationary treatment of the anisotropic component of the distribution function has been used in the study of microwave conductivity (Viehland et al., 1988). Essentially all theoretical analysis of electron swarms in ac fields prior to the 1990s involved the two-term Legendre polynomial expansion of the velocity distribution function in velocity space and expansion in Fourier series in time.

In the late 1980s and early 1990s, the combined Legendre-Fourier treatment initially developed by Margenau and Hartman (1948) has been extended and employed by Makabe and Goto (1988), Goto and Makabe (1990), Ferreira et al. (1991), Loureiro (1993) and Sa et al. (1994) to investigate the temporal variation of the isotropic component of the velocity distribution function. The works of Makabe and Goto (1988) and Goto and Makabe (1990) deserves special mention. First, these works were developed with the principal aim of analyzing the applicability of time resolved swarms data in interpretation of measurements for rf plasmas. Second, in contrast to previous techniques for solving the Boltzmann equation, the effects of non-conservative collisions (ionization/attachment) on time-dependent electron kinetics were considered. In particular, the time-resolved ionization and attachment rate coefficients in CH₄, H₂ and their mixtures have been examined. Third, Goto and Makabe (1990) extended their previous work (Makabe and Goto, 1988) to consider the first solutions beyond the two-term limit in ac electric fields. Practically, however, in their approach to solve the spatially homogeneous Boltzmann equation, the Legendre-Fourier expansions were generally restricted to low order approximations in both l and k indices and hence their technique from the nowadays point of view is of limited applicability. A salient feature of their technique, as pointed out by White et al. (2002) was a trade off between accurate representation of the temporal structure and accuracy in the transport coefficient amplitudes.

In summary we may identify the following restrictions and inadequacies among various techniques for solving the Boltzmann equation for charged particle swarms in ac fields prior to the early 1990s:

- Theories were restricted to low-order truncations in the Legendre expansions of the velocity dependence (quasi-isotropy in velocity space). This in turn had implications on the types of gases and field amplitudes which could be considered. In other words, an accurate solution of the Boltzmann equation was possible only for atomic gases in low $E/n_0$ range.
• Theories had imposed restrictions on the range of applied frequencies.

• The Boltzmann equation was solvable for spatially homogeneous systems only. In other words, the study of spatially inhomogeneous swarm transport coefficients in ac fields remained unexplored until the mid-1990s.

• Theories were generally restricted to electron swarms.

• Theories were able to consider the electron swarms under the action of time-dependent electric field only. In other words, the theories were unable to treat charged particle swarms when both the electric and magnetic ac fields are present.

In order to improve the accuracy of the time-dependent treatment of the electron kinetics, the first multi-term solutions of the Boltzmann equation under spatially homogeneous conditions were independently developed at the James Cook University in Townsville (Australia) (White, 1993) and Institute of Low Temperature Plasma Physics in Griefswald (Germany) (Loffhagen and Winkler (1996a; 1996b)). The group at the Keio University in Yokohama (Japan) applied the so-called direct numerical procedure (DNP), initially developed by Drallos and Wadehra (1988; 1989), to solve the Boltzmann equation under spatially homogeneity (Maeda and Makabe (1994a; 1994b)). These groups were able to overcome accuracy, field frequency and gas type restrictions associated with many other techniques for solving the Boltzmann equation.

Time-dependent multi-term solutions of the Boltzmann equation under spatially inhomogeneous conditions developed at the James Cook University in Australia represent an important step forward (White et al. (1995); White (1996)). The group at the Keio University extended their approach to solve the Boltzmann equation based on the DNP to consider the spatially inhomogeneous swarms (Maeda et al., 1997). Also in the mid-1990s, the group at the Institute of Physics in Belgrade developed a Monte Carlo simulation technique which was used to study the spatially inhomogeneous electron swarms in rf fields. Many complex kinetic phenomena in electron transport underlying the application of plasma processing in rf fields have become the new focus of attention of the three latter mentioned groups. In particular, since the study of spatially inhomogeneous swarm transport coefficients in ac fields remained completely unexplored, much efforts have been invested by these three groups in order to understand the behavior of the diffusion tensor and its diagonal elements in ac electric fields. Perhaps the most notable phenomenon observed by these groups is that of “anomalous anisotropic diffusion”. As remarked previously, in dc swarms, the phenomenon of anisotropic diffusion was observed in the late 1960s and explained theoretically using the Boltzmann equation analysis by Parker and Lowke (1969a; 1969). It was found that for majority of gases the transverse diffusion coefficient dominates the longitudinal diffusion coefficient for a wide range of electric field strengths. These unusual results were verified in many experimental measurements. In rf fields, however, it was found recently that the time dependence of electron diffusion coefficients shows anomalous behavior for the longitudinal component of the diffusion tensor (White et al. (1995); White (1996); Maeda et al. (1997)). The anomaly is reflected in the following: firstly, the longitudinal diffusion coefficient peaks during or just after the phases when the electric field changes the sign, second, for a brief
phase period, the longitudinal diffusion coefficient becomes larger than the transverse diffusion coefficient. In addition, the effect has been observed in crossed time-dependent electric and magnetic fields (Raspopović et al., 2000), where longitudinal as well as transverse components along the $\mathbf{E} \times \mathbf{B}$ direction of the diffusion tensor show anomalous behavior. Apart from being an interesting kinetic phenomenon that cannot be explained by a dc theory, the anomalous behavior of the longitudinal diffusion occurs at the moment when the field becomes zero and may create a strong flux of electrons along the direction of the electric field. So far such flux has not been taken into account in fluid models of rf plasmas and it is not quite certain how well such flux would be represented in particle codes. Generally speaking, the correct representation of the diffusion coefficients is of great importance for applications in the diffusion controlled breakdown of gases, maintenance of rf discharges and fluid modeling of rf plasma discharges. In this thesis, we will discuss in detail the anomalous nature of some diagonal elements of the diffusion tensor in time-dependent electric and magnetic fields for certain model and real gases.

Another example which falls into the category of kinetic phenomena in electron transport in ac fields and which has been investigated employing the Boltzmann equation is that of “time-resolved negative differential conductivity”. The first presentation of the time-resolved negative differential conductivity has been done for methane by Goto and Makabe (1990) who employed, as mentioned above, the combined Legendre-Fourier treatment for solving the Boltzmann equation. The first rigorous multi-term Boltzmann analysis of this phenomenon has been presented by White (1996). Using a Monte Carlo simulation technique, the theoretical observations made through the Boltzmann equation analysis have been verified by Jelenak et al. (1995), Petrović et al. (1997) and Bzenić et al. (1999). In dc fields, it is well-known fact that for some gases the drift velocity decreases over a range of $E/n_0$ values as the field is increased. In rf fields, it was observed that NDC exists over a certain phase of the field at low frequencies. As the field frequency increases, the asymmetric temporal profile of the drift velocity is developed and then in the limit of high frequency the effect of NDC is entirely removed. Apart from being an interesting kinetic phenomenon that cannot be explained in terms of conventional dc theory, the NDC effect in rf fields has implications for the power deposited into the plasma. In this thesis, the time-resolved NDC is studied for CF$_4$ and argon-CF$_4$ mixtures.

Another class of kinetic phenomena in ac fields is associated with the explicit effects of non-conservative collisions. As discussed recently by Petrović et al. (2002) and White et al. (2002), the effects of non-conservative collisions on electron transport can be quite large under the appropriate conditions. Of particular note was the observed ‘phase-lead’ associated with the drift velocity profile (i.e. the drift velocity changes the sign before the field changes sign) when attachment processes play an important role (White et. al. (1999b; 2002)). However, perhaps the most striking kinetic phenomena induced by the presence of the attachment processes is that of negative absolute electron mobility in ac fields Dujko et al. (2003). It was shown that the distinction between bulk and flux drift velocities is not just in the opposite directions but also in a large phase delay introduced for the bulk drift velocity. Šuvakov et. al. (2005) pointed out that the positive value of the bulk mobility and its delay in rf fields may be explained by a wave of localized attachment that changes the center of mass of the electron swarm. The
phenomenon was observed in a gas mixture of argon and molecular fluorine under conditions which led to negative electron mobility in the afterglow-dc field conditions. As discussed by Petrović et al. (2002), this phenomenon may be of relevance for certain regions of rf plasmas, where the effective field may be low and at the same time typical mixtures used in plasma processing are those that show the negative mobility effect. At the more fundamental level, the thermodynamic study of Robson et al. (2003) actually points out that the total entropy of the system increases as evidenced by the positive bulk drift velocity. One should bear in mind that it is only the bulk drift velocities that are measured in standard swarm experiments. However, if some property depending on the flux drift velocity only can be identified then one may be able to point out a way to either observe the negative mobility or even to use it.

Recent developments in plasma processing using magnetically controlled/assisted rf plasma discharges have led to a resurgence of interest in electron kinetics in rf electric and magnetic fields. Large classes of non-equilibrium plasma devices utilize electromagnets, permanent magnets or induced magnetic fields with the goal of enhancing plasma density or improving electron confinement (Makabe and Petrović (2006); Makabe and Maeshige (2002)). Hence one of the most challenging areas in plasma modeling is an accurate representation of the effects of a magnetic field on charged particle kinetics. However, in most cases, the effect of a magnetic field on electron transport is being neglected, or at best effective field approximations are being applied. On the other hand, a recent extension of some standard plasma models by Kushner and co-workers (Sankaran and Kushner (2002); Vasenkov and Kushner (2003a; 2003b)) to include $E \times B$ effects and time-resolved electron kinetics has led to a better understanding of the power transfer to ICPs. Similar attempts have been made by Makabe and co-workers in a different geometry (Tadokoro et al., 1998). In general however, temporal non-locality of electron transport in time-dependent electric and magnetic fields has not been the subject of special studies or inclusion in plasma models.

In contrast to the extensive literature on electron swarms in dc electric and magnetic fields, until recently very little has been carried over to electron swarms in ac electric and magnetic fields. In that respect, the recent work of the group at the Institute of Physics in Belgrade (Serbia) deserves special mention. In their work, the effects of time resolved magnetic field on rf electron transport were systematically studied by a Monte Carlo simulation technique for the most common configuration found in plasma reactors—an orthogonal configuration of electric and magnetic fields where the fields are $\pi/2$ out of phase (see for example Petrović et al. (2002); Raspopović et. al. (2000; 2005); Šašić et. al. (2007; 2009)). Their Monte Carlo technique has given rise to a whole new dimension of new physical phenomena. A similar program has been carried out at the James Cook University in Townsville (Australia) and in order to achieve this goal, a general and accurate theory was required. Such a theory, in crossed ac electric and magnetic fields based on the spherical harmonics decomposition of the Boltzmann equation has been recently published by White et al. (2002). A Monte Carlo simulation technique was used to test this theory and it was found that theory is valid under conditions when electrons undergoing conservative collisions only (White et al., 2007). One of the principal aims of this thesis is to make a further generalization of this theory and consider the explicit effects of non-conservative
collisions under conditions of arbitrary field orientation and phase differences between the fields. We have observed a multitude of kinetic phenomena that are generally inexplicable through the use of steady-state dc transport theory. We systematically study the origin and mechanisms for such phenomena, their sometimes paradoxical manifestation and possible physical implications which arise from their explicit inclusion into plasma models. As an illustrative example, a proposed new mechanism for collisional heating in ICP has emerged from this thesis.

1.4 Some factors in the historical development of the Boltzmann equation analysis under non-hydrodynamic conditions

1.4.1 Non-hydrodynamic phenomena in transport of charged particles

In recent years the study of spatially resolved electron kinetics in neutral gases under the action of electric and magnetic fields has gained in importance for development and further optimization of plasma sources used in plasma processing industry (Makabe and Petrović, 2006). One of the major challenges in this area is an understanding of the spatial variations and related relaxation processes of the electron transport properties in atomic and molecular gases. This essentially non-hydrodynamic behavior is often labeled in physics of non-equilibrium plasmas as non-local (or transient) behavior. The concept of “non-local electron kinetics” was pioneered by Bernstein and Holstein (1956) and Tsendin (1974). It is usually dealt with by employing Monte Carlo based hybrid approaches or Particle in Cell (PIC) modeling. As such non-local behavior usually develops in plasmas in the region of the rapid changes of electric field, it is necessary to test the models and interpretations against uniform field, swarm type experiments and models. This is the program carried out in this thesis.

The spatial variations of the electron transport properties can be caused by various mechanisms. These include the local disturbances of the electron velocity distribution function, electron transport in rapidly varying fields in space, the presence of external sources of ionization, electron transport at very high electric field to gas number density ration ($E/n_0$) or electron transport near emitting or absorbing physical boundaries such as electrodes, enclosing walls, internal grids and probes. A number of theoretical methods to calculate the electron transport properties under these “non-hydrodynamic” conditions, especially those attempting to model or simulate the cathode fall of a dc (Boeuf and Marode, 1982) or sheath of rf discharges (Kim et al., 1999), revealed the non-local nature of electron transport. The failure of the hydrodynamic approximation and the spatial non-locality of electron transport have been recognized and marked as one of the biggest difficulties in the early development of plasma models (Petrović et. al. (2002; 2007)). A survey of various kinetic problems and difficulties occurring in inhomogeneous plasma regions, their approximate kinetic treatment and range of applicability prior the 1990s has been reviewed in (Kortshagen et. al. (1996b; 2002)).

The first experimental observations of non-hydrodynamic phenomena in electron transport date back to the 1920s. The seminal experiment of Franck and Hertz, as discussed recently by
Robson et al. (2000) and Sigeneger et al. (2003), was the first to provide evidence of these effects, while Holst-Oosterhuis periodic luminous layers observed in rare gas discharges are also a manifestation of such phenomena (Holst and Oosterhuis, 1921). Holst and Oosterhuis observed a series of alternate dark and luminous layers in the prebreakdown region of a plane-parallel discharge in neon with currents of about 10 µA at low values of $E/n_0$ of about 20 Td. The layer next to the cathode was perfectly dark and was followed by a sharply limited luminous layer. Similar observations of luminous layers were reported by Grotrian (1921), Penning (1926; 1931), Druyvesteyn (1932), Chanin and Rork (1963; 1964), Hayashi (1982) and Fletcher (1985). Another well-known example of typical non-hydrodynamic behavior of the electrons in conventional dc discharges is the occurrence of striations. Several types of striations in rare gases have been identified and classified but in general they appear due to the connection between ionization rate and electron number density. This connection is different for atomic and molecular gases and depends on the operating conditions. Striations were first observed and recorded in notebooks by Faraday while the first description of the striations has been published by Abria (1843). The accumulated knowledge about striations was recently reviewed by Kolobov (2006). However, in spite of these well-known illustrative examples, the spatial variations and associated relaxation phenomena of the electron transport properties have been difficult to quantify experimentally on a systematic basis because of their dependence on initial and experimental conditions (Pitchford et al., 1990). Moreover, in the swarm experiments used for measurement of the electron transport coefficients and determination of low energy electron-molecule cross sections, both theoretical and experimental work has been carried out to avoid/minimize the detrimental action of non-hydrodynamic phenomena in order to obtain more reliable hydrodynamic transport properties (Kumar et al., 1980). One such example is separation of the delay distance and the hydrodynamic exponential growth in SST experiments and analysis of Paschen curve (Malović et al., 2003) or measurement of excitation coefficients.

1.4.2 Techniques of solving the Boltzmann equation under non-hydrodynamic conditions

The major players in the early development of non-hydrodynamic kinetic theory were Morse and co-workers (Morse et al., 1935), Holstein (1946) and Bernstein and Holstein (1956). In particular, the work of Bernstein and Holstein (1956) deserves more mention. Their work concerned electron kinetics in a space charge electric field and they developed a method which relies on the direct solution of the electron Boltzmann equation. Their method was further advanced by Tsendin (1974) and forms the basis of the so-called nonlocal approach and local field approximation (Tsendin (1995); Kortshagen et. al. (1996b; 2002)). The main idea behind the nonlocal approach is that the entire electron kinetics can be represented by a single, spatially homogeneous electron total energy distribution function, which is determined from a spatially averaged kinetic equation. In other words, the nonlocal approach finds a solution of a spatially averaged kinetic equation, and reduces the space-dependent description of the electron kinetics to an effectively one-dimensional problem. The space dependence of the electron distribution function is derived from a “generalized Boltzmann relation” in the nonlocal method. Two im-
portant limitations are associated with this approach: first, the “nonlocal approach” applies
strictly only to the confined electrons, i.e., those electrons which have a total energy too low
to overcome the space charge potential in order to escape to the discharge walls; and second,
this method is valid only when electron energy relaxation length exceeds dimensions of spatial
inhomogeneity (Kortshagen et al. (1996b; 2002); Li (1999)). In contrast to nonlocal approach,
the local field approximation is frequently employed under conditions of high pressures. In the
local field approximation, the electron transport properties can be well approximated by their
local field values, which are hydrodynamic calculated for the same magnitude of the field as the
space-dependent field at the specific location in space. However, when transport properties are
dependent upon global spatial information of the electric field, the local electric field is insuffi-
cient to represent transport properties, and a full non-local field consideration must be made.
In other words, the local field approximation is valid when the characteristic dimension \( L \) of
plasma non-uniformity exceeds the electron energy relaxation length \( \Lambda_e \), \( L \gg \Lambda_e \). Although
the local field approximation is not valid for classic discharge physics problems such as a cathode
sheath of glow discharge or the positive column of dc discharge at low pressure, it is interesting
to note that this approach has been more frequently employed in plasma modeling community
than the nonlocal approach (Kortshagen et al., 1996b). For example, the validity of the local
field approximation in both free space and plasma discharges has been examined by a number
of investigations (see, e.g., Sato and Tagashira (1985), Moratz et al. (1987), Segur et al. (1995),
Sigeneger and Winkler (1995)). However, the general validity of the nonlocal approach for
collision-dominated plasma has been demonstrated in a number of experimental and theoretical
investigations (see Kortshagen et al. (1996b; 2002) and references therein).

Within the framework of non-hydrodynamic kinetic theory, the seventies were notable for
the works of Whipple and Parker (1971), Bender and Muller (1973), Lyagushchenko (1973),
Lowke et al. (1977), Sakai et al. (1977) and Segur and Keller (1977). In a self-consistent model-
ing of plasma diodes, Whipple and Parker (1971) investigated the spatially resolved electron and
ion kinetics by integrating the Boltzmann equation for Maxwell type of elastic collisions. Bender
and Muller (1973) employed a two-term approximation in Legendre polynomials to study the
electron kinetics in a spatially inhomogeneous electric field. Neglecting the energy loses in elas-
tic collisions, the analytical solution of the Boltzmann equation was found. They demonstrated
that striations occurred in a spatially periodic electric field appear as eigenfunction solutions of
electron motion in a homogeneous electric field. Lyagushchenko (1973) applied a two-term the-
ory to investigate the spatial relaxation of the distribution function under field free conditions.
He showed that the distribution function in field free conditions relaxes monotonically to a spa-
tially uniform state, with a relaxation length controlled by elastic collision processes. Lowke et
al. (1977) employed a two-term approximation in Legendre polynomials to solve the Boltzmann
equation under conditions of a spatially uniform electric field. Their program was to study the
behavior of the distribution function and other transport properties near the boundaries. It
was observed that near the boundary the distribution function is space-dependent and hence as
pointed out by Lowke and co-workers the concept of diffusion coefficients and drift velocity is not
valid under conditions of large density gradients. They proposed that under non-hydrodynamic
conditions the key transport quantity should be the distribution function. Sakai et al. (1977) employed a two-term theory for solving the Boltzmann equation under different physical conditions, e.g. they solved the Boltzmann equation under pulsed Townsend (PT), time of flight (TOF) and steady-state Townsend (SST) conditions when non-conservative collisions are operative. It was shown that the value of a transport property is dependent on the type of experiment, even when the value of \( E/n_0 \) is kept the same. Finally, Segur and Keller (1977) developed a numerical method of solving the Boltzmann equation under non-hydrodynamic conditions relying upon the concept of characteristic lines. In this method, motion of charged particles are described by characteristic lines in configuration and total energy spaces and the Boltzmann equation is solved directly by numerical integration. Their method was further improved and employed for solving the Boltzmann equation under conditions of both spatially homogeneous and spatially inhomogeneous electric fields (Segur et. al. (1983; 1983b; 1984; 1995)). Considerable contributions in this field have been made by Tsendin (1982a; 1982b) and Popov et al. (1993) who also observed periodic variations in the isotropic distribution function and some other transport properties of the electrons with spatial positions.

In understanding physically the spatial variations of the electron transport parameters, the propagator method initially developed by Sommerer et al. (1989) and the steady-state Townsend flight time integral (SST-FTI) method have also played an important role. Sugawara and co-workers improved the propagator method of Sommerer et al. (1989) and applied this method for calculation of SST spatially uniform electron transport properties (Sugawara et. al. (1992; 1994)). This technique is somewhat similar to the particle in cell (PIC) method which is widely used in plasma physics. The trajectories are processed in a similar way to that of the Monte Carlo method but no random processes are used for the collisions. However, although the idea of this technique is very interesting, it suffers from the numerical diffusion problem as some traditional numerical methods for solving the Boltzmann equation. The SST-FTI method has been employed for the similar studies of spatially resolved energy distribution function and electron transport properties in CF\(_4\) (Takeda and Ikuta, 1997).

More recently, the modern non-hydrodynamic kinetic studies on the electron spatial relaxation revealed the complex nature of the relaxation process and associated basic mechanisms. The groups at Griefswald (Winkler and co-workers) and James Cook University (Robson and co-workers) attract special attention. Unlike others, who directly applied their methods to treat complex plasma phenomena in various inhomogeneous plasma regions, they focused on the half-range free space problems including the modeling of an idealized steady-state Townsend experiment with the aim of understanding fundamental mechanisms of spatial relaxation of electron ensemble properties. Winkler and co-workers employed a two-term, Legendre polynomial representation of the velocity distribution for solving the Boltzmann equation to study the field free spatial relaxation of the electrons and related spatially decaying plasma phenomena (Winkler and Sigeneger, 2001), spatial relaxation of the electrons in uniform (Winkler et. al. (1996; 1997); Sigeneger and Winkler (1997a; 1997b)) and non-uniform (Loffhagen et al., 2003) electric fields, spatial relaxation in spatially periodic fields (Sigeneger et. al. (1998; 2000); Sigeneger and Winkler (1995; 2000)) and response of the electrons to spatial disturbance of the electric field
A two-term representation of the distribution function in spherical harmonics has been applied for a treatment of both the non-local electron kinetics in the anode region (Arndt et al., 2000) and radially inhomogeneous electron kinetics (Uhrlandt and Winkler, 1996), and for the description of the radially and axially varying non-local electron kinetics in a cylindrical dc plasma configuration (Arndt et al., 2001). The two-term theory has been extended to a multi-term treatment of spatial relaxation in spatially uniform fields (Petrov and Winkler, 1997), and spatial relaxation in the cathode (Petrov and Winkler (1998); Hannemann et al. (2000)) and anode (Loffhagen et al., 2002) regions of a glow discharge. Similar kinetic studies on spatial relaxation of the electrons in uniform and spatially periodic fields have been performed by Golubovskii et al. (1998; 1999; 2000; 2002). For atomic systems, it may be anticipated that the two-term analysis is of sufficient accuracy, but in general, a multi-term representation of the distribution function, in full spherical harmonics, not just Legendre polynomials, is required (White et al., 2003). This was the program carried out by Robson and co-workers in an attempt to study the effects of non-conservative collisions on spatial relaxation of the electrons Li et al. (2002), using a two-temperature moment method, whereby the spatial dependence was treated by both finite difference and eigenfunction techniques. However, the spectrum of problems associated with spatial relaxation processes of the electrons is even larger. In that respect, the effect of electron-electron interactions (Loffhagen, 2005) and effects of a magnetic field (Winkler et al. (2000); Li et al. (2006); White et. al. (2006; 2008)) on spatial relaxation of the electrons have been investigated.

In the past the kinetic treatment of time-dependent problems has been largely restricted to spatially uniform plasma configurations while the instantaneous and/or local electric field approximations were used to investigate the electron kinetics in a space and time varying electric field. Nowadays, it is well known that a spatiotemporal treatment of electron kinetics is indispensable for understanding the non-equilibrium behavior of the electrons in plasmas. First attempts to solve the kinetic equation of the electrons including both the space and time dependence have been reported by Goedheer and Meijer (1993) and by Mahmoud and Yousfi (1997). Goedheer and Meijer (1993) investigated the spatiotemporal description of the electron kinetics in a 1-dimensional rf discharge plasma between plane electrodes, while Mahmoud and Yousfi (1997) have focused their efforts on the spatiotemporal development of an electron swarm in weakly ionized gases. A two-term representation of the distribution function in Legendre polynomials and the quasi-stationary description of the anisotropic part of the distribution function have been employed in these studies. Similar but not identical approach was used by Loffhagen and Winkler (2001), Winkler et al. (2002) and Winkler et al. (2004) for the description of the spatiotemporal relaxation of electrons in the column-anode plasma of a glow discharge. Note that a comprehensive multi-term theory appropriate to deal with the spatiotemporal relaxation of the electrons in neutral gases is still missing.

In addition to half-range free space problems associated preferentially with the fundamental relaxation phenomena and elementary processes, one ought to mention the recent self-consistent non-hydrodynamic studies on electron kinetics in various inhomogeneous plasma regions. There are many published papers in this field, but we briefly review contributions that are impor-
tant in the context of the theory presented in this thesis. For example, Alves et al. (1997) developed self-consistent formulation to solve the steady-state spatially inhomogeneous electron Boltzmann equation in a plasma positive column, taking into account the spatial gradient and the space-charge field terms. The problem is solved in cylindrical geometry using the two-term approximation in Legendre polynomials, with appropriate boundary conditions for the electron velocity distribution function, especially at the tube wall. Their formulation is self-contained in the sense that the electron particle balance equation is exactly satisfied, that is, the ionization rate exactly compensates for the electron loss rate to the wall. Passoth et al. (1999) employed a two-term approximation to solve the spatially inhomogeneous Boltzmann equation in order to study the radial behavior of the EDF in the cylindrical magnetron discharge in argon. Their method was further improved by Porokhova et. al. (2001; 2002; 2003). They developed a self-consistent kinetic model of plasma in the entire gap of a magnetron cylindrical discharge where all quantities vary along the radial and axial directions. The discharge modeling is performed on the basis of a numerical solution of the spatially inhomogeneous Boltzmann kinetic equation together with equations of ion motion, current balance, and Poissons equation. The model represents an example of discharge description from cathode to anode with respect to strong non-locality effects in the distribution function formation. The self-consistent hybrid models recently developed by the group at the Institute for Low-temperature Plasmas in Greifswald (Germany) are of special note. These hybrid methods have been used for a self-consistent analysis of a helium plasma in a cylindrical hollow cathode (Sigeneger and Winkler, 2005), for a self-consistent analysis of the spatial relaxation of the EDF and densities of excited atoms induced by a disturbance caused by a floating Langmuir probe (Arndt et al., 2005) and for the self-consistent studies of the anode region of a glow discharge (Arndt et al., 2003).

In particular, the recent work of Porokhova and co-workers on modeling magnetron discharges deserves special mention. They developed a multi-term approach for cylindrical magnetron discharges in crossed electric and magnetic fields (Porokhova et al., 2005a) extending the previously developed non-hydrodynamic multi-term analysis for an electric field only (Robson et al., 2002) and the hydrodynamic transport theory when both fields are present (Ness, 1993). In many aspects they applied the same theoretical ideas and mathematical machinery employed in this thesis. The same multi-term kinetic approach was then applied to model the electron component of an argon magnetron discharge (Porokhova et al., 2005b) and as remarked recently by Li et al. (2006), this work represents the most comprehensive and the most sophisticated kinetic study of a magnetron plasma discharge to date.

In what follows, we wish to emphasize the importance of the previous studies by Winkler and co-workers and Robson and co-workers in the context of a program carried out in this thesis. The conclusions emerging from the previous studies of the Winkler and co-workers and Robson and co-workers in the case of an electric field only are consistent with each other and may be summarized as follows. The nature of the spatial relaxation profiles of the electron transport properties is dependent on the interplay between the power dissipated in elastic collisional processes, power dissipated in threshold collisional processes and the power dissipated into the swarm by the field (Li (1999); Robson et al. (2000); Li et al. (2002); Winkler et al. (2002)). For
certain gases, there exist a “window” of $E/n_0$ strengths where the relaxation profiles are damped oscillatory in nature, and outside this window the profiles are monotonic. Li et al. (2002) have considered the explicit effect of ionization on the spatial relaxation profiles of the electron transport properties. They have observed and explain an increase in the period of oscillation due to the explicit effects of ionization. However, we have observed that an error exists in the results presented in the same reference arising from an incorrect numerical implementation of the boundary at infinity in the computer code. As an illustrative example, the presented spatial profiles for the mean energy, average velocity and ionization rate for the ionization model of Lucas and Saelee are incorrect. Thus we have been motivated to re-consider this problem and to remove any misunderstandings associated with the physical explanation of the spatial relaxation of electrons in an idealized SST experiment when non-conservative collisions are operative.

Another issue that is highly relevant for plasma modeling is the spatial relaxation of the electrons in electric and magnetic fields. As remarked previously, the motivation for the present work is provided by the recently published papers of Winkler et al. (2000) and Li et al. (2006), in which the effect of a magnetic field orthogonal to an electric field on the spatial relaxation behavior of the electron velocity distribution and electron transport properties is investigated. They have observed that when a magnetic field is present, a “window” of $E/n_0$ strengths where the relaxation profiles are damped oscillatory in nature can be shifted while the relaxation profiles, including the modulation amplitude, relaxation length and period of oscillations of the electron transport properties can be significantly modified. Winkler et al. (2000) employed a two-term, Legendre polynomial representation of the velocity distribution for solving Boltzmann’s equation for electrons in neon while Li et al. (2006) employed a multi-term representation of the distribution function in full spherical harmonics for solving the Boltzmann equation for electrons in methane and for certain model gases. It is important to note that a program of investigation carried out by Li et al. (2006) was based on a two temperature moment method, whereby the spatial dependence was treated by both finite-difference and eigenfunction techniques. In particular, it has come to the attention of the authors of the same reference that the computer code contains an error associated with the implementation of a finite-difference method for solving the Boltzmann equation. This fact was second motivation factor for us to develop an accurate non-hydrodynamic theory and associate numerical codes to investigate the spatial relaxation of various transport properties of the electrons in an idealized SST experiment. We approach the problem at two stages: firstly, a Monte Carlo simulation technique to consider the spatial relaxation of the electrons in an idealized SST experiment under the influence of electric and magnetic fields crossed at arbitrary angle when non-conservative collisions are present is developed. More about this code will be outlined in the next section. Secondly, a multi-term solution of the conservative Boltzmann equation has been developed and used to investigate the spatial relaxation of charged-particle swarms under the influence of electric and magnetic fields in a crossed field configuration. We employ a ‘two-temperature’ Burnett function representation of operators in velocity space in the Boltzmann equation while the configuration space is represented by pseudo-spectral and finite difference methods for certain model gases.
1.5 A brief sketch of Monte Carlo simulation technique under hydrodynamic and non-hydrodynamic conditions

Monte Carlo (MC) method is one of the main approaches of ‘computer simulation’ in statistical and plasma physics. This method is now recognized as an important tool to solve a variety of physical problems complementing both analytical theory and experiment. MC method can be distinguished from other simulation methods (such as molecular dynamic simulation) by being stochastic. In all applications of the Monte Carlo method, a stochastic model is constructed in which the expected value of a certain random variable is equivalent to the value of a physical quantity to be determined. The expected value is then estimated by the average of multiple independent samples. For the construction of the series of independent samples, the random numbers are used. In practice, of course, these numbers are not truly random but rather are ‘pseudo-random numbers’ i.e. a sequence of numbers produced on a computer with a suitable deterministic procedure (see section 7.3).

Historically, the idea of using random numbers in the calculation of deterministic quantities was first introduced by von Neumann and Ulam (see Forsythe and Leibler (1950); von Neumann (1951)) for the tasks of multi-dimensional integration and matrix inversion. The last author is credited with suggesting the term ‘Monte Carlo simulation’ (with reference to the well known gambling house). For the case of charged particle transport in neutral gases, the first references are the works of Itoh and Musha (1960) and Skullerud (1968). Itoh and Musha developed a MC method to estimate the ionization coefficient $\alpha/p_0$ and drift velocity $W$ for three values of $E/p_0$ in helium. Two important aspects of this work must be emphasized. In this work the electron orbit was approximated by a series of continuous segments each of which has a length equal to a tenth of the mean free path at the appropriate electron energy. At the end of a segment a uniform pseudo-random number $\xi$ between zero and unity was generated, and the occurrence of collision was judged. It was assumed that a collision occurred if $\xi < 0.1$. If there is no collision the mean free path corresponding to the energy of the electron at the end of the segment is calculated and the procedure repeats. Therefore, in this work Itoh and Musha demonstrated the first accurate solution of the equation for the collision probability between electron and background neutral molecule. Secondly, in this work the ergodic hypothesis was assumed to estimate the mean energy of the electrons, i.e. it was assumed that the behavior of a single electron sampled a large number of times was the same as the behavior of all the electrons at any time. This procedure is only strictly valid for a volume where the mean properties are not influenced by the electron diffusion and non-conservative collisions. Hence the method of Itoh and Musha may therefore be subject of errors of the same order as those calculated using the spatially homogeneous Boltzmann equation when non-conservative collisions are treated simply as other inelastic processes.

Skullerud’s paper in 1968 represents the introduction of the so-called “Null collision method”. Development of this method was driven by a need for a simple and fast method for determining the free time between two ‘successive’ collisions for a charged particle moving through a background gas under the influence of an electric field where the collision frequency is energy
dependent. This approach introduces a null species such that in a charged particle-null species collision the charged particle velocity does not change. The cross section for the charged particle-null species collision is chosen to obtain a constant total collision frequency allowing analytical solution of the equation for the collision probability (see section 5.5). Further optimizations and computationally efficient implementations of Skupperud’s null collision technique were proposed by Lin and Bardsley (1977), Reid (1979) and Brennan (1991). Generally speaking, the null collision technique was introduced to remove one of the greatest sources of arbitrariness in the MC technique, and that is the choice of the length of the time segments required for a numerical treatment of the electron motion between two successive collisions. It also improves the speed and reliability of the codes.

In an attempt to overcome the limitations of the ergodic hypothesis, Thomas and Thomas (1969) developed a MC method in which all the electrons belonging to a swarm were followed so that the electron diffusion in the configuration space and the effects of non-conservative collisions were properly taken into account. In this work, Thomas and Thomas (1969) demonstrated the first exact calculation of the ionization coefficient by a Monte Carlo method. Similar MC approach was employed by Folkard and Haydon (1970) in their study on non-equilibrium effects at high values of $E/n_e$ in hydrogen. Generally speaking, during the 1970s and early 1980s, a MC method has been provided a means of examining a great number of phenomena that were either difficult or impossible to analyze with other available methods. These phenomena include: boundary effects (Burch and Wheaton (1977); Tran et al. (1977); Braglia and Lowke (1979); Oluchi and Kubota (1983)); spatial relaxation of the electrons and other related non-hydrodynamic phenomena (Hayashi (1982); Segur et al. (1983b)); electron transport greatly influenced by non-conservative processes (Lucas and Saelee (1975); Penetrante and Bardsley (1983)); effects of anisotropic scattering on electron transport (Saelee and Lucas (1977); Blevin et al. (1978); Kunhardt and Tzeng (1986)); electron thermalization in gases (Koura (1983; 1984; 1985; 1986a; 1986b; 1987a; 1987b)) and the development of the gas discharges (Kline and Siambis (1972); Kunhardt et al. (1986); Kunhardt and Tzeng (1988)). In addition, one of the main motivating factors behind Monte Carlo simulations have been to serve as an independent check on the accuracy and reliability of various techniques for solving the Boltzmann equation (Sakai et al. (1977); Reid (1979); Reid and Hunter (1979)).

The work of Tagashira’s group deserves more mentioning. This group has demonstrated the differences in the electron transport properties due to the methods of observation, pulsed Townsend (PT), steady-state Townsend (SST) and time of flight (TOF) following the previous work of Thomas (1969) and proposed the way of sampling of spatially resolved electron transport data under SST conditions (Sakai et al. (1972; 1977)). This formalism was followed by Boeuf and Marode (1984) to study the spatially resolved electron transport properties in SF$_6$ (1984) and non-hydrodynamic effects in the electron transport within the cathode region of a glow discharge (Boeuf and Marode, 1982). The spatial structures in excitation coefficients in the SST experiment in the vicinity of cathode in nitrogen have been studied by Kelly et al. (1989). The behavior of electrons under the influence of spatially inhomogeneous electric field has been studied by Sato and Tagashira (1985) and Moratz et al. (1987).
Although MC simulations have been extensively used in 1970s for a wide range of problems as mentioned previously, they established themselves as a powerful simulation tool during the 1980s. This was initially driven by the need for accurate drift and diffusion coefficients for electrons in gases and gas mixtures used in gas lasers and (Kukukarpaci and Lucas (1979); Kukukarpaci et al. (1981)) and in wire-chamber detectors (see Blum and Rolandi (1993) and reference therein). Since there were no experiments set up to measure these transport coefficients, theoretical calculations were the only other option. In particular, Fraser and Mathieson (1987a; 1987b) developed a MC method for the determination of electron transport properties in counting gases used in particle detectors. Unfortunately, the swarm and particle detector communities lost their contact over the years and many parallel studies have been made (Petrović et al., 2002). As an illustrative example, Fraser and Mathieson (1987a; 1987b) revealed the anisotropic nature of the diffusion in argon-methane gas mixtures which was a well known fact in the swarm community from the beginning of 1970s.

Early MC work on the motion of electron swarms in electric and magnetic fields has been presented by Razdan et al. (1985). A MC method has been employed to investigate the effect of a transverse magnetic field on electron transport under the action of non-uniform electric field in a cathode fall of a glow discharge. It has been shown that the application of a magnetic field reduces the instabilities of a discharge which was of great importance to improve the performance of some gas lasers. The influence of a transverse magnetic field on electron energy distribution function and other transport properties in SF$_6$ by a MC method has been investigated by Govinda Raju and Dincer (1985), Dincer (1993) and Milsom (1993). In a similar fashion, a MC method has been employed to evaluate the swarm parameters in nitrogen (Govinda Raju and Dincer, 1990), mercury vapor (Liu and Govinda Raju, 1992) and CO$_2$ (Xu et al. (1994)). In 1990, Brennan et al. (1990) carried out MC simulations of electron swarms in molecular nitrogen for perpendicular electric and magnetic fields in order to assist with the interpretation of data from “photon-flux” experiments. This paper represents the first study of spatially-resolved electron transport data in crossed electric and magnetic fields. The common motivating factors behind these studies include the stabilization and optimization of gas laser discharges and magnetically controlled high-voltage switches. By solving the collision-less equation for the electron motion in $E \times B$ fields and employing the null collision technique, these authors evaluated the electron swarm parameters as a function of the electric and magnetic field strengths. More recently, Nakamura et al. (1999) employed a MC method to study the electron transport in crossed electric and magnetic fields in argon and methane while Liu et al. (2000) investigated the electron transport processes in positive column of a helium dc discharges under conditions of parallel fields. In addition, one ought to mention the recent Monte Carlo studies of electron transport in a channel region of a stationary plasma thruster (Latocha et al., 2002) and Monte Carlo modeling of the behavior of electrons and ions in an argon hollow-cathode discharge under the influence of a transverse or longitudinal magnetic field (Lai et al., 2000).

During the 1980s and 1990s the number of MC simulations used for electron swarm in dc electric and magnetic fields rapidly increased in response to increasing awareness of the limitations of the two-term approximation for solving the Boltzmann equation. The main motivating
factors have been to probe the limitation of the two-term approximation and to serve as an independent check on the accuracy and reliability of the increasing number of multi-term Boltzmann equation solutions. For example, Penetrante et al. (1985) employed the MC method for the Reid ramp model and methane while Yachi et al. (1988; 1991) and Itoh et al. (1988; 1990) carried out MC simulations for the same gases and SF$_6$ in order to test their multi-term theory for solving the Boltzmann equation under the PT, SST and TOF conditions. Kortshagen et al. (1996a) employed a MC code to test the validity of the nonlocal approach for solving the spatially dependent Boltzmann equation for electron in low-pressure plasma discharges. In 1997, White et al. (1997) carried out benchmark MC simulations of electron swarms in perpendicular electric and magnetic fields for a range of conservative model gases as an independent check on the multi-term solution of Ness (1994) and the “flight time integral” (FTI) method of Ikuta and Sugai (1989). Biagi (1999) has developed a MC simulation code for electron swarms in electric and magnetic fields, primarily for determination of transport parameters in counting gas mixtures. The most recent version of the MAGBOLTZ contains a database of 58 gases, whose properties are known with varying accuracy. The output data of Biagi’s MAGBOLTZ include the attachment and ionization rate coefficients, drift velocity components, Lorentz deflection angle and diagonal elements of the diffusion tensor. Note that Biagi’s code cannot compute the flux transport coefficients and off-diagonal elements of the diffusion tensor. Perhaps the main disadvantage of Biagi’s code lies with the fact that the cross sections are stored internally, hard-coded directly into the program so modifying the cross sections requires finding and parsing the proper subroutine within approximately $3 \times 10^4$ lines of FORTRAN. The same MC code has been used to test numerical integrity of a multi-term theory for solving the Boltzmann equation for electric and magnetic fields crossed at arbitrary angle (White et al., 1999a).

Aside from the effects of a dc magnetic field upon the electron transport, there are many other phenomena important for the understanding of electron kinetics in plasma discharges, analyzed by a MC method. The illustrative examples include the studies of the effects of electron-electron collisions on electron transport (Weng and Kushner (1990); Alkaa et al. (1994)), the effects associated with the energy partition after an ionizing event on the velocity distribution function (Tzeng and Kunhardt, 1986), the effects of a strong electron attachment in electronegative gases on electron transport parameters when both hydrodynamic (Yousfi et al., 1994) and non-hydrodynamic (Dyatko and Napartovich, 1999) conditions are operative, the effects of anisotropic electron scattering on the electron transport properties (Kunhardt and Tzeng (1986); Vasenkov (2000)), the breakdown mechanism in rf fields from diffusion to multipacting controlled conditions (Gilardini, 1999), the insulation characteristics of gases (Wu et al. (2006); Liu et al. (2008)) and many other which will be mentioned in later chapters. However, one of the main motivating factors behind the MC analysis of the electron transport is the determination of low-energy electron-molecule cross sections. As discussed previously, this can be done through the so-called inversion procedure where the cross sections are adjusted until some preset agreement is obtained between experimentally measured and calculated transport coefficients by a MC method or alternatively by solving the Boltzmann equation. A number of papers has been published in this area but the standard references for this technique are the books of Huxley.
and Crompton (1974) and Mason and McDaniel (1988). More recent results can be found in
the review papers of Crompton (1994) and Petrović et al. (2007).

Perhaps one of the most frequent applications of a Monte Carlo simulation technique can be
found in the field of low-temperature plasmas modeling (Bruno et. al. (2003)). It is well known
fact however, that a Monte Carlo method describes the transport properties of charged particles
in neutral gases and usually cannot be used for a self-consistent description of plasma discharge.
A glaring exception is a self-consistent Monte Carlo simulation technique developed by Lawler
and Kortshagen (1999) which has been applied for investigation of the positive column of a glow
discharge. In general, due to the complexity and multidimensionality of the kinetic equations,
many authors have incorporated a Monte Carlo method in their numerical codes to study a wide
range of plasma phenomena. As already remarked, the hybrid plasma models utilize a Monte
Carlo method for a treatment of ‘non-equilibrium’, fast electrons while the ions and heavy
particles are usually treated by a fluid approach. As an illustrative example, Donko employed
a one-dimensional hybrid approach based on a Monte Carlo method to describe the transient
behavior of low-pressure discharges in argon (Donko, 2000) and two-dimensional hybrid approach
to study the low-current self-generated oscillations in a rectangular hollow cathode discharge
in helium (Donko, 1999). Hybrid codes based on a Monte Carlo method together with proper
inclusion of the effects of a magnetic field have led to a better understanding of the power transfer
to the ICPs (Tadakoro et al. (1998); Vasenkov and Kushner (2003a; 2003b)). Another class of
plasma codes widely used within plasma modeling community is a Particle in Cell/Monte Carlo
(PIC/MC) method (see for example Tskhakaya et al. (2007) and references therein). PIC/MC
simulation has been of interest with many scientific and technological applications. To name a
few: modeling of plasma thrusters (Garrigues et al., 2000) which are well adapted for satellite
station keeping, modeling of a magnetron discharges (Shidoji et al. (1999; 2001); Kondo and
Nanbu (1999); Nanbu et al. (1996; 2000); Liebermann and Lichtenberg (1994)) which are mostly
used in the deposition of thin films and modeling of CCP (Yan and Goedheer, 1999) and ICP
(Oh and Makabe (2000); Takeida and Nanbu (2005)) which are widely used in plasma processing
industry.

The initial version of a Monte Carlo simulation code used in this work was developed at
the Institute of Physics in Belgrade (Serbia). A wide spectrum of problems associated with the
charged particle transport in gases has been attacked with this code. Under non-hydrodynamic
conditions, the code has been employed to investigate the electron transport at very high values
of $E/n_0$ (Stojanović and Petrović, 1998) when both runaway and boundary effects are significant
throughout discharge. The same Monte Carlo code has been used to model the spatial distribu-
tion of excitation when heavy particle excitation dominates electron excitations by more than
two orders of magnitude (Stojanovic et al. (1997); Petrović and Stojanović (1998)). The same
group has carried out many parallel MC studies on the electron transport when hydrodynamic
conditions prevail. The code has been employed for the comprehensive studies of negative elec-
tron mobility in dc (Dyatko et al., 2000) and rf fields (Dujko et al., 2003), kinetic phenomena
in rf fields such as anomalous anisotropic diffusion (Maeda et al., 1997) and time-resolved neg-
ative differential conductivity (Bzenić et al., 1999), temporal relaxation of distribution function
in rf fields (Bzenić et al., 1999), benchmarking in dc and rf fields (Raspopović et al., 1999) and for many other important aspects of plasma modeling. In addition, one ought to mention the recent Monte Carlo studies on non-conservative transport of positrons in neutral gases (Šuvakov et al. (2008); Banković et al. (2008)) by the same group. However, one important aspect of the Belgrade group which is of great relevance for the studies in the framework of this thesis deserves special mention. They applied a Monte Carlo simulation technique in order to study non-conservative electron transport in crossed rf electric and magnetic fields under conditions which can be found in ICP reactors (see for example theses of Bzenić (1997); Raspopović (1999); Sakadžić (2000) and Dujko (2004)), monograph of Dujko (2005) and the following references Petrović et al. (2002); Raspopović et al. (2000; 2005) and Šasić et al. (2007; 2009)). These studies have unearthed a wide range of kinetic phenomena, i.e. phenomena that cannot be directly extrapolated either from steady-state dc results or from individual particle trajectories. At the same time, these studies provide benchmarks for plasma models in the limit of low electron density.

In the present work we extend the initial version of the code developed at the Institute of Physics in Belgrade by introducing some new elements. First, the code initially developed at the Institute of Physics in Belgrade has been improved to treat the swarms in an infinite space under the combined action of electric and magnetic fields crossed at arbitrary angle. In addition, the code has been further improved to follow and sample spatially resolved characteristics along the swarm. We employ where possible the infrastructure associated with the previous version of the code which has been built up, to produce a more comprehensive code suitable for general treatment of non-conservative electron transport in electric and magnetic fields crossed at arbitrary angles. The resulting code has been tested against similar calculations and found to be correct. The results of testing are presented in this thesis. In addition, the new improved code has been employed in a recent study on non-conservative electron transport in CF\textsubscript{4} in electric and magnetic fields crossed at arbitrary angle (Dujko et al. (2005; 2006)). This thesis does not have room for the presentation of these results.

A non-trivial extension of the Monte Carlo code to consider the spatial relaxation of the electron swarm under the influence of electric and magnetic fields crossed at arbitrary angle under steady-state conditions in infinite plane-parallel geometry has been developed. Calculations have been performed for electron transport properties with the aim of providing benchmarks required to verify the codes in plasma modeling. Both the spatially uniform values and relaxation profiles of the electron transport properties may serve as an accurate test for other codes. The explicit effects of ionization and attachment on the spatial relaxation profiles are considered using physical arguments. We identify the relations for the conversion of hydrodynamic transport properties to those found in the steady-state Townsend (SST) experiment. Our Monte Carlo simulation code and sampling techniques appropriate to these experiments has provided us with a way to test these conversion formulae and their convergence. We identify some inaccuracies or oversimplifications in basic definitions of the transport coefficients and numerical approaches to their calculation in MC simulations. The synergism of magnetic fields and non-conservative collisions on spatial relaxation profiles associated with various electron transport properties is
1.6 Scope and structure of the thesis

Below we give a short description of the contents of the various parts of this thesis.

In Chapter 2 the language of irreducible tensors is introduced since it is extensively used throughout the thesis. The time-dependent hydrodynamic and steady-state non-hydrodynamic regimes are discussed followed by definitions of the transport properties for an arbitrary field configuration. The velocity dependence of the phase-space distribution function is then represented in terms of spherical harmonics. Considering different spatial conditions in these two regimes, space dependence of the distribution function is further treated separately. In the time-dependent hydrodynamic regime the spatial dependence of the phase-space distribution function is treated using an instantaneous second order density gradient expansion. The Boltzmann equation for a swarm of charged particles is decomposed into a hierarchy of kinetic equations for the moments of the distribution function. The symmetry properties of the Boltzmann equation and the distribution function (and its moments) and their consequences on the transport coefficients in time-dependent electric and magnetic fields are investigated. Expressions are given for the hydrodynamic spatially homogeneous distribution function and transport coefficients in the presence of non-conservative collisions in terms of the time-dependent moments. In the steady-state non-hydrodynamic regime, the spatial dependence of the phase-space distribution function is retain intact during the decomposition process of the Boltzmann equation. The resulting hierarchy of partial differential equations is discussed. Transport properties including the number density, mean energy and average velocity components when electric and magnetic fields are crossed at arbitrary angle are given in terms of the spatially dependent moments of the distribution function.

In Chapter 3 the speed dependence of the phase-space distribution function under hydrodynamic and non-hydrodynamic conditions is treated through an expansion in terms of Sonine polynomials about a Maxwellian at an arbitrary basis temperature. Under conditions of the time-dependent hydrodynamic regime, an implicit finite-difference scheme in time is employed and the resulting hierarchy of coupled inhomogeneous matrix equations is given. The explicit form of both the bulk and flux transport coefficients and other transport properties is given in a Sonine polynomial basis. For the steady-state non-hydrodynamic regime however, the resulting system of equations represents a system of coupled ordinary differential equations for the moments of the distribution function. Expressions for various transport properties under non-hydrodynamic conditions are given in a Sonine polynomial basis. In this chapter, the matrix elements of the various collisional operators from the interaction potentials (for ions) and partial cross sections (for electrons) in the Burnett function basis are determined. The matrix elements are given in terms of the interaction integrals for an arbitrary order in the mass ratio.

Chapter 4 summarizes the computational algorithms adopted to solve the hierarchy of coupled inhomogeneous matrix equations for the time-dependent moments under hydrodynamic
conditions. The internal scheme for the determination of the basis temperature at each time step and iterative scheme for the determination of the reaction rate are addressed. A system of coupled ordinary differential equations for the moments of the distribution function derived for non-hydrodynamic conditions is numerically solved using the pseudo-spectral and finite difference method. The main numerical restrictions associated with these techniques are also indicated.

Chapter 5 details a Monte Carlo simulation technique employed in this thesis. In this chapter we describe in detail how the path of an individual electron in electric and magnetic fields is simulated and how the exact moment and nature of of the next collisions are determined. A new scheme to calculate the expansion coefficients in density gradient expansions of average transport properties in the hydrodynamic regime is developed and used to represent the SST transport properties in terms of these general quantities. The sampling techniques for spatially dependent electron transport data are used to calculate these hydrodynamic expansions under SST conditions and to test their convergence and range of applicability.

In Chapter 6 we investigate the numerical accuracy of the present theory and code using the Reid ramp model and non-conservative model gases in electric and magnetic fields crossed at arbitrary angle. A comparison of the results of the Monte Carlo method with those of a multi-term Boltzmann equation analysis shows good agreement. Results are given for electron swarms over a range of angles between the fields and field strengths. The errors associated with the two-term approximation and inadequacies of Legendre polynomial expansion procedure for solving the Boltzmann equation are highlighted.

In Chapter 7 the hydrodynamic kinetic theory and Monte Carlo simulation code developed in previous chapters are employed to investigate the temporal relaxation of the electrons under the influence of electric and magnetic fields crossed at arbitrary angle when electron transport is greatly influenced by non-conservative collisions. We employ a series of model and real gases to study the various relaxation phenomena. Certain trends in the temporal relaxation profiles of the electron transport coefficients are addressed using physical arguments.

In Chapter 8 the hydrodynamic kinetic theory and Monte Carlo simulation code are employed to investigate the electron transport coefficients and other transport properties in ac electric and magnetic fields for certain model and real gases. We focus on the time-dependent behavior of electron transport properties under conditions which can be generally found in magnetically controlled/assisted rf discharges. We systematically investigate the explicit effects associated with the electric and magnetic fields including field to density ratios, field frequency, field phases and field orientations. No restrictions is placed on the magnitude or frequency of the applied electric and magnetic fields. The studies uncover a multitude of kinetic phenomena that are generally inexplicable through the use of steady-state dc transport theory. Phenomena of significant note include the existence of transient negative diffusivity, time-resolved negative differential conductivity and anomalous anisotropic diffusion. In particular, in this chapter we propose a new additional mechanism for collisional heating in rf electric and magnetic fields caused by the synergism of temporal non-locality and cyclotron resonance effect.
Finally, in Chapter 9 the non-hydrodynamic kinetic theory for solving the spatially dependent Boltzmann equation in association with a Monte Carlo simulation technique is employed to investigate the spatial relaxation of electrons in an idealized SST experiment. The synergism of magnetic field effects and non-conservative collisions on spatial relaxation of the electrons is investigated using both model and real gases, here argon and CF$_4$ as an illustrative example.
Chapter 2

Spherical harmonic decomposition of the Boltzmann equation

2.1 Introduction

The starting point for most modern-day solutions of Boltzmann’s equation is the decomposition of the charged particle phase space distribution function in terms of spherical harmonics in velocity space. The spherical harmonics expansion has to do with the velocity space only, and applies to both hydrodynamic and non-hydrodynamic conditions. The general formalism for the spherical harmonic decomposition of the Boltzmann equation for charged particle swarms in the presence of non-conservative collisions (ionization/attachment) in neutral gases under the action of dc electric field was developed by Robson and Ness (1986). The further extension of this formalism includes the works of Ness (1993) and White (1996). Ness (1993) presented a formal theory based upon the spherical decomposition of the charged particle phase space distribution function for swarms in neutral gases in the presence of uniform and static electric and magnetic fields crossed at arbitrary angle. Extension of the kinetic theory for swarms in ac electric fields has been investigated by White (1996) and White et al. (1998; 1999b). By combining the formalism of Ness (1993) and White (1996), White et al. (2002) developed the first multi-term solution of the conservative Boltzmann equation based on a spherical harmonics decomposition of the velocity distribution function. In this chapter, the contribution of White et al. (2002) is further generalized to consider the presence of non-conservative collisions. No assumptions are made concerning the number of spherical harmonics in the spherical harmonic decomposition.

The second step in decomposing the Boltzmann equation is a treatment of the spatial dependence of the distribution function and its moments. The spatial representation of the distribution function must be treated differently within the hydrodynamic and non-hydrodynamic theory. In the time-dependent hydrodynamic theory, the spatial dependence is treated by assuming a time-dependent hydrodynamic regime. The time-dependent hydrodynamic regime requires that system has evolved to a stage where the spatial dependence of the distribution function and
its moments are linear functionals of the number density. Obviously, this is a generalization of dc hydrodynamic theory and its validity and correctness has been recently investigated by White et al. (1999b) under conditions of time-dependent electric fields. Working with the irreducible tensor-algebra, the Boltzmann equation is decomposed into a hierarchy of coupled time-dependent kinetic equations. The inclusion of the time-dependent magnetic field results in a change of form of the kinetic equations to those associated with the steady-state regime and the specific configuration of ac electric field only and these modifications are highlighted. In order to describe the effects of non-conservative collisions on the diffusion coefficients, the second order density gradient expansion is required.

However, under non-hydrodynamic conditions, such a density gradient expansion procedure is no longer valid, and the space and velocity dependence must be treated on an equal footing. In this chapter, the space dependence of the distribution function is retained explicitly throughout the entire decomposition process of the Boltzmann equation. In later chapters, the spatial dependence of the distribution function and its moments are treated through the appropriate numerical schemes.

The number density of a swarm of charged particles is assumed to be much less than that of the neutral background molecules and the only collisions influencing the swarm of charged particles are those with neutral species. The charged particle-neutral molecule interactions are assumed to proceed via central forces while the distribution of neutral molecule velocities is spatially uniform, stationary and isotropic in velocity space. We assume the neutral background molecules remain in thermal equilibrium and their internal states are characterized by a Boltzmann distribution. The applied electric and magnetic fields are assumed to be uniform in space. In the framework of hydrodynamic studies, the applied fields are assumed to be time-dependent while non-hydrodynamic study presented here concerns dc electric and magnetic fields. No restrictions are made with respect to the form of this time-dependence, however, in the subsequent chapters the focus is on a sinusoidal form of both the electric and magnetic fields.

Solution of the hierarchy of kinetic equations (whatever the spatial representation) yields the distribution function components and all the transport properties. In case of the time-dependent hydrodynamic regime, this solution yields the hydrodynamic distribution function components and all transport coefficients and properties of interest. The definition and physical interpretation of transport coefficients for an arbitrary configuration of time-dependent electric and magnetic fields in the presence of non-conservative collisions is discussed in the context of a time-dependent hydrodynamic description. In addition, the structure and symmetries among the elements of the vector and tensorial transport coefficients for different field configurations is studied.

2.2 Mathematical background: Algebra of irreducible tensors

The mathematical machinery behind the kinetic theory developed in this thesis is based upon the algebra of irreducible tensors. The tensor formalism and convention in this thesis is set out
in detail by Fano and Racah (1959), in the papers of Kumar (1966a; 1967) and in the references Robson and Ness (1986) and Ness (1993). The same convention was applied in the theses of Robson (1972), Ness (1985), White (1996) and Li (1999). We follow these previous works but only essential definitions, properties and theorems will be given here.

The irreducible tensors are defined with respect to rotations of a three dimensional coordinate frame. They can be standard or contrastandard. A contrastandard irreducible tensor of rank $l$, is a set of $(2l+1)$ objects which transform under rotations of the coordinate frame like a spherical harmonic

$$Y_{m}^{l}(\theta, \phi) = i^{l}(-1)^{(m+|m|)/2} \left[ \frac{(2l+1)(l-|m|)!}{4\pi(l+|m|)!} \right]^{1/2} P_{l}^{m}(\cos \theta)e^{im\phi}. \quad (2.1)$$

where the associated Legendre polynomials are defined by

$$P_{l}^{m}(\cos \theta) = \frac{(-1)^{l}}{2^{l}l!} (\sin \theta)^{|m|} \frac{d^{l+|m|}}{d\cos \theta^{l+|m|}} (1-\cos^{2}\theta)^{l}. \quad (2.2)$$

The corresponding standard tensor is simply the complex conjugate and is denoted by

$$f_{m}^{(l)} = f_{m}^{(l)*}. \quad (2.3)$$

Tensors of the same rank and standardization can be further distinguished through the additional superscript (e.g. $T_{m}^{[l]}$).

Any two standard/contrastandard irreducible tensors can be coupled to produce another standard/contrastandard irreducible tensor according to the prescription

$$T_{m}^{(l)} = \left[ a^{(l_{1})}, b^{(l_{2})} \right]^{(l)}_{m} = \sum_{m_{1}m_{2}} (l_{1}m_{1}l_{2}m_{2}|lm) a_{m_{1}}^{(l_{1})}b_{m_{2}}^{(l_{2})}, \quad (2.4)$$

where the sum is over all allowed values of $m$ indices and $(l_{1}m_{1}l_{2}m_{2}|lm)$ is a Clebsch-Gordan or Wigner coefficient which vanishes unless $m_{1} + m_{2} = m$ and $l_{1} + l_{2} \geq l \geq |l_{1} - l_{2}|$. Various properties and identities of these Clebsch-Gordan coefficients are given in standard texts on angular momentum theory (Condon and Shortley (1953); Rose (1957); Fano and Racah (1959); Sakurai (1966a; 1967); Varshalovich et al. (1988)). Using the orthogonality of Clebsch-Gordan coefficients

$$\sum_{lm}(l_{1}m_{1}l_{2}m_{2}|lm)(l_{1}m'|l_{2}m'|lm) = \delta_{m_{1}m'}\delta_{m_{2}m'}, \quad (2.5)$$

the inverse coupling rule is given by

$$a_{m_{1}}^{(l_{1})}b_{m_{2}}^{(l_{2})} = \sum_{lm}(l_{1}m_{1}l_{2}m_{2}|lm) T_{m}^{(l)} . \quad (2.6)$$

When two spherical harmonics of the same arguments are coupled, the result is another spherical harmonic (Kumar (1966b))

$$Y_{m_{1}}^{l_{1}}(\theta, \phi)Y_{m_{2}}^{l_{2}}(\theta, \phi) = \sum_{l} \sigma(l_{1}l_{2}l)(l_{1}m_{1}l_{2}m_{2}|l_{1}m_{1} + m_{2}) Y_{m_{1}+m_{2}}^{l_{1}}(\theta, \phi), \quad (2.7)$$

where

$$\sigma(l_{1}l_{2}l) = i^{l_{1}+l_{2}-l} \left[ \frac{(2l_{1}+1)(2l_{2}+1)}{4\pi(2l+1)} \right]^{1/2} (l_{1}0l_{2}0|l_{1}l_{2}l). \quad (2.8)$$
Another useful relation associated with the spherical harmonics is their orthogonality relation
\[
\int Y^l_m(\theta, \phi)Y^{l'}_{m'}(\theta, \phi)d(\cos \theta)d\phi = \delta_{ll'}\delta_{mm'} .
\] (2.9)

The velocity vector \( \mathbf{c} \), and operators \( \nabla \) and \( \partial/\partial \mathbf{c} \) play important role in the decomposition of the Boltzmann equation. If we define the spherical vector
\[
c^{[1]}_m = \sqrt{\frac{4\pi}{3}}cY^{[1]}_m(\hat{\mathbf{e}}) ,
\] (2.10)
where \( \hat{\mathbf{e}} \) denotes the angles of the velocity \( (\theta, \phi) \), then the connection between Cartesian and spherical components of the velocity vector is given by
\[
c_x = \frac{i}{\sqrt{2}} \left[ c^{[1]}_1 - c^{[1]}_{-1} \right]
\]
\[
c_y = \frac{1}{\sqrt{2}} \left[ c^{[1]}_1 + c^{[1]}_{-1} \right]
\]
\[
c_z = -ic^{[1]}_0 .
\] (2.11)

Likewise, the gradient tensor operators in configuration and velocity space are related to their Cartesian counterpart components via (Kumar, 1967)
\[
\nabla_0^{[1]} = i \frac{\partial}{\partial z} \\
\nabla_{\pm 1}^{[1]} = \frac{1}{\sqrt{2}} \left( \mp i \frac{\partial}{\partial x} + \frac{\partial}{\partial y} \right) \\
\partial^{[1]}_{c\pm 1} = \frac{1}{\sqrt{2}} \left( \mp i \frac{\partial}{\partial c_x} + \frac{\partial}{\partial c_y} \right) .
\] (2.12)

The corresponding standard tensors can be found directly from these expressions.

The spherical form of higher order configuration space gradient operators is required in the expansion of the spatial dependence of certain quantities. Robson and Ness (1986) introduced the gradient tensor operator \( G^{(s l)}_m \):
\[
G^{(00)}_0 = 1 \\
G^{(11)}_m = \nabla^{(1)}_m \quad (m = 0, \pm 1) \\
G^{(2l)}_m = \left[ G^{(11)}_m, G^{(11)}_m \right]^{(l)}_m \quad (m = 0, ..., \pm l), (l = 0, 2) .
\] (2.13)

In general however,
\[
G^{(s l)}_m = \left\{ \begin{array}{ll} 0 & \text{if } l > s \text{ or } |m| > l \\ 0 & \text{if } s + l = \text{odd} \end{array} \right. 
\] (2.14)

The last restriction results from the independence of the order of coupling of the first rank tensors. In addition, like spherical harmonics, the gradient operator must satisfy
\[
G^{(s l)}_m = \left( G^{(s l)}_m \right)^* = (-1)^{l-m}G^{(s l)}_{-m} .
\] (2.15)

The operation \( * \) denotes complex conjugation. Examples of the relation of the gradient operator to its cartesian operator counterparts is given in Table 2.1.
Table 2.1: Cartesian components of the gradient tensor operator.

<table>
<thead>
<tr>
<th>$s$</th>
<th>$l$</th>
<th>$m$</th>
<th>$G_{m}^{(st)}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0</td>
<td>0</td>
<td>1</td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td>0</td>
<td>$-i\partial_{z}$</td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td>$\pm 1$</td>
<td>$\pm i\partial_{x} + \partial_{y}$</td>
</tr>
<tr>
<td>2</td>
<td>0</td>
<td>0</td>
<td>$\nabla^{2}$</td>
</tr>
<tr>
<td>2</td>
<td>2</td>
<td>0</td>
<td>$\sqrt{\frac{2}{3}} \left[ \frac{1}{2} (\partial_{x}^{2} + \partial_{y}^{2}) - \partial_{z}^{2} \right]$</td>
</tr>
<tr>
<td>2</td>
<td>2</td>
<td>$\pm 1$</td>
<td>$\pm i\partial_{x} - i\partial_{y}$ $\partial_{z}$</td>
</tr>
<tr>
<td>2</td>
<td>2</td>
<td>$\pm 2$</td>
<td>$\pm i\partial_{x} + \partial_{y}$ $\partial_{z}$</td>
</tr>
</tbody>
</table>

In later sections parity operations are used to investigate symmetries and it is useful at this stage to introduce the identities:

$$
\left( G_{m}^{(s\lambda)} \right)^{\dagger} = (-1)^{s} G_{m}^{(s\lambda)} \tag{2.16}
$$

$$
Y_{m}^{[l]}(-\hat{c}) = (-1)^{l} Y_{m}^{[l]}(\hat{c}), \tag{2.17}
$$

where the symbol $\dagger$ denotes the operation $r \rightarrow -r$.

Finally, if $T_{\mu}^{[\lambda]}$ is an irreducible tensor which depends on $c$ and the differential operator $\partial/\partial c$, then the Wigner-Eckart theorem is

$$
\int Y_{m_{1}}^{(l_{1})}(\hat{c}) T_{\mu}^{[\lambda]} Y_{m_{2}}^{(l_{2})}(\hat{c}) = \langle l_{1}m_{1}|T_{\mu}^{[\lambda]}|l_{2}m_{2} \rangle \\
= \langle l_{2}m_{2}\lambda\mu|l_{1}m_{1} \rangle < l_{1}||T^{[\lambda]}||l_{2} >, \tag{2.18}
$$

where $\langle l_{1}||T^{[\lambda]}||l_{2} >$ is referred to as the reduced matrix element (Kumar (1967); Robson and Ness (1986)).

### 2.3 Hydrodynamic and non-hydrodynamic regimes

The experimentally measurable quantities are usually the charged particle current or charged particle densities $n(r,t)$ instead of the phase-space distribution function. The connection between experiment and theory is usually made through the equation of continuity

$$
\frac{\partial n(r,t)}{\partial t} + \nabla \cdot \Gamma(r,t) = S(r,t), \tag{2.19}
$$

where $\Gamma(r,t) = n < c >$ is the swarm particle flux and $S(r,t)$ represents the production rate per unit volume per unit time arising from non-conservative collisional processes. The number
density of the charged particles \( n(r, t) \) is defined by

\[
n(r, t) = \int f(r, c, t) dc .
\] (2.20)

The equation of continuity describes the change in \( n(r, t) \) due to a flux of the swarm particles \( \Gamma(r, t) = n < c > \) and production term \( S(r, t) \). This equation is valid for both hydrodynamic and non-hydrodynamic regimes and represents the starting point in development of a theory presented in this thesis.

### 2.3.1 The time-dependent hydrodynamic regime and definitions of transport coefficients

Far from boundaries, sources and sinks, the hydrodynamic regime is assumed to apply. In the time-dependent hydrodynamic regime the space-time dependence is entirely carried by the density \( n(r, t) \) of charged particles and the distribution function has the form

\[
f(r, c, t) = \sum_{k=0}^{\infty} f^{(k)}(c, t) \odot (-\nabla)^k n(r, t) ,
\] (2.21)

where \( f^{(k)}(c, t) \) are time-dependent tensors of rank \( k \) and \( \odot \) denotes a \( k \)-fold scalar product. Note that in (2.21) there is an additional explicit source of time-dependence in addition to the implicit dependence associated with the number density. The domain of the validity of the representation (2.21) under time-dependent conditions has been recently discussed (White et al., 1999b).

Assuming the functional relationship (2.21), the flux \( \Gamma(r, t) \) and source term \( S(r, t) \) in (2.19) are expanded as follows:

\[
\Gamma(r, t) = \sum_{k=0}^{\infty} \Gamma^{(k+1)}(t) \odot (-\nabla)^k n(r, t) ,
\] (2.22)

\[
S(r, t) = \sum_{k=0}^{\infty} S^{(k)}(t) \odot (-\nabla)^k n(r, t) ,
\] (2.23)

where the superscript \( (k) \) and \( (k+1) \) denote the ranks of the tensors and \( \odot \) denotes the appropriate tensor product. Equation (2.22) represents the generalized time-dependent flux-gradient relation. Truncation of the expansion at \( k = 1 \) gives

\[
\Gamma(r, t) = W^{(*)}(t)n(r, t) - D^{(*)}(t) \cdot \nabla n(r, t) ,
\] (2.24)

where \( W^{(*)}(t) \) and \( D^{(*)}(t) \), define, respectively, the flux drift velocity and flux diffusion tensor. Substitution of expansion (2.22) and (2.23) into the continuity equation (2.19) yields the generalized time-dependent diffusion equation

\[
\frac{\partial n(r, t)}{\partial t} = \sum_{k=0}^{\infty} \omega^{(k)}(t) \odot (-\nabla)^k n(r, t) ,
\] (2.25)
\[ \omega^{(k)}(t) = \Gamma^{(k)}(t) - S^{(k)}(t) \]  

(2.26)

Truncation of (2.25) at \( k = 2 \) yields the time-dependent diffusion equation,

\[ \frac{\partial n}{\partial t} + W(t) \cdot \nabla n - D(t) : \nabla \nabla n = -R_a(t)n , \]  

(2.27)

which define the bulk transport coefficients

\[
\begin{align*}
R_a(t) &= -\omega^{(0)}(t) = S^{(0)}(t) \\
W(t) &= \omega^{(1)}(t) = W^{(*)}(t) + S^{(1)}(t) \\
D(t) &= \omega^{(2)}(t) = D^{(*)}(t) + S^{(2)}(t)
\end{align*}
\]

(2.28)

(2.29)

(2.30)

To gain further insight into the physical meaning of the time-dependent transport coefficients, we take the spatial moments of the number density. Pre-multiplying the generalized continuity equation (2.25) by an arbitrary function \( \psi(r) \) and integrating over all configuration space, the time-dependent transport coefficients can then be expressed as time-dependent time derivatives of these moments:

\[
\begin{align*}
R_a(t) &= -\omega^{(0)}(t) = \frac{d}{dt} \left( \log N(t) \right)(t) \\
W(t) &= \omega^{(1)}(t) = \frac{d}{dt} \langle r(t) \rangle(t) \\
D(t) &= \omega^{(2)}(t) = \frac{1}{2} \frac{d}{dt} \left( r(t) - \langle r \rangle(t) \right) \left( r(t) - \langle r \rangle(t) \right) ,
\end{align*}
\]

(2.31)

(2.32)

(2.33)

where

\[
\begin{align*}
N(t) &= \int n(r,t)dr \\
\langle \psi(r) \rangle(t) &= \frac{1}{N(t)} \int \psi(r)n(r,t)dr .
\end{align*}
\]

(2.34)

(2.35)

The quantity \( R_a(t) \) is the time-dependent loss rate. We can give a physical interpretation for the bulk drift velocity \( W(t) \) as the time-dependent velocity of the center-of-mass of the swarm. From (2.33), the tensor quantity \( D(t) \) represents the time-dependent rate of change of the mean square width of the swarm or equivalently the time-dependent rate of spreading of the swarm. The analogy with the dc case (Kumar et al., 1980) is clearly evident.

The basic difference between the bulk and flux transport coefficients should now be apparent. It follows from (2.32) that the bulk drift velocity is displacement of the mean position of the electron swarm and it characterizes the motion of the total ensemble of electrons. The presence of the electric field results in a spatial variation in the energy throughout the swarm (White, 1996). Under such conditions, the presence of non-conservative collisions (ionization/attachment) may lead to a change in the position of the center-of-mass of the swarm. This effect on the bulk drift velocity is denoted by \( S^{(1)}(t) \). On the other hand, the flux drift velocity \( W^{(*)}(t) \) represents the rate of change of the position of the center-of-mass due to the electric field only. It can be interpreted as the mean velocity of the electrons. Likewise the flux diffusion tensor \( D^{(*)}(t) \) represents the rate of spreading of the swarm due to \( E \) and \( \nabla n \). The presence of non-conservative
collisions may result in the variation of the $\nabla n$ throughout the swarm and a subsequent variation in the rate of change of the mean squared width of the swarm. Such effects are expressed by the second rank tensor $S^{(2)}(t)$. Obviously, in the absence of non-conservative collisions the $S^{(k)}$ source/sink terms describing the production/loss of electrons vanish and the bulk and flux transport coefficients coincide.

In swarm experiments it is generally the bulk transport coefficients which are measured and tabulated (Robson et al., 2005). There are no experiments for measuring the flux transport coefficients but in many aspects of plasma modeling these transport coefficients are required. The differences between, and implications associated with, the two sets of transport coefficients will be discussed in later chapters.

Another important issue is to consider the structure of vector and tensor transport coefficients in electric and magnetic fields. If it is not specified differently, in this thesis we consider a co-ordinate system in which the $z$ axis is defined by the electric field $E$ while the magnetic field $B$ makes an angle $\varphi$ with $E$ and lies in the $y-z$ plane. For this general configuration, the vector and tensorial transport coefficients and other transport properties are generally full (White et al. (1999a; 2002)). In particular, this means that there are three independent components of the drift velocity vector and nine independent components of the diffusion tensor and they have the following form:

$$W = \begin{pmatrix} W_x \\ W_y \\ W_z \end{pmatrix}; \quad D = \begin{pmatrix} D_{xx} & D_{xy} & D_{xz} \\ D_{yx} & D_{yy} & D_{yz} \\ D_{zx} & D_{zy} & D_{zz} \end{pmatrix}. \quad (2.36)$$

In contrast to an arbitrary configuration of the electric and magnetic fields, for parallel and orthogonal field configurations tensors are sparse and symmetries exist among the elements. In case of parallel field configuration, the rotational invariance and parity imply the drift velocity vector and diffusion tensor must have the following form:

$$W = \begin{pmatrix} 0 \\ 0 \\ W_z \end{pmatrix}; \quad D = \begin{pmatrix} D_{xx} & D_{xy} & 0 \\ D_{-xy} & D_{xx} & 0 \\ 0 & 0 & D_{zz} \end{pmatrix}. \quad (2.37)$$

while for orthogonal fields they reduce to the well-known form (Ness (1993)):

$$W = \begin{pmatrix} W_x \\ 0 \\ W_z \end{pmatrix}; \quad D = \begin{pmatrix} D_{xx} & 0 & D_{xz} \\ 0 & D_{yy} & 0 \\ D_{zx} & 0 & D_{zz} \end{pmatrix}. \quad (2.38)$$

It must be emphasized that other transport properties with the same tensorial rank have the similar structure.

### 2.3.2 Non-hydrodynamic regime and definitions of transport properties

As we mentioned previously, under large gradient spatially inhomogeneous conditions the hydrodynamic assumption in development of theory is invalid. In such a case the transport properties
of a swarm of charged particles are space-dependent. While the continuity equation (2.19) still holds, the diffusion equation (2.25) (under dc conditions) is no longer valid simply because a low order density gradient expansion is not sufficient under such conditions (Li, 1999).

Figure 2.1: Schematic representation of the idealized steady-state Townsend experiment. Charged particles emitted at a constant rate from an infinite plane source at \( z = z_0 \) interact with the background neutral gas under static external electric and magnetic fields and evolve downstream \( z \geq z_0 \).

In this thesis we consider an idealized SST experiment with plane-parallel geometry, as shown schematically in figure 2.1. A plane source emits charged particles with charge \( q \) at a steady rate into an infinite gas between anode and cathode under the influence of electric and magnetic fields crossed at arbitrary angle. The electric field is oriented along the \( z \)-axis while magnetic field lies in \( z-y \) plane making an angle \( \psi \) with \( z \)-axis.

Under these conditions, there exists a steady-state in which properties are independent of time and vary with the position only in the \( z \)-direction. The Boltzmann equation has the following form:

\[
 c_z \frac{\partial}{\partial z} f(z,c) + \frac{q}{m} \left [ E + c \times B \right ] \frac{\partial f(z,c)}{\partial c} = -J(f,f_0) ,
\]

where \( m \) is mass of the swarm particle, \( f(z,c) \) is the particle distribution function at coordinate \( z \) and velocity \( c \) and \( J \) is the linear collision operator describing charged-particle-gas-molecule interaction. Therefore, in configuration space, this is a one-dimensional problem with \( z \) as a variable in the distribution function.

The main quantities of physical interest are those which can be measured in the experiments under non-hydrodynamic conditions. These include the number density, mean energy, average velocity and non-conservative collision rate. Their definitions are given by respectively

\[
n(r) = \int f(r,c) dc ,
\]

\[
\epsilon(r) = \frac{1}{n(r)} \int \frac{1}{2} mc^2 f(r,c) dc ,
\]

\[
v(r) = \frac{1}{n(r)} \int cf(r,c) dc ,
\]

\[
51
\]
\[ R(r) = \frac{1}{n(r)} \int J^R f(r, c) dc. \] (2.43)

where \( J^R \) is the collision operator describing the non-conservative collision processes. It should be noted that the average velocity in (2.42) corresponds to the flux velocity.

### 2.4 Spherical harmonics decomposition of the Boltzmann equation

#### 2.4.1 Expansion of the velocity distribution function

The phase-space distribution function is a time-dependent scalar function of the position and velocity vectors \( r \) and \( c \) respectively. Thus we can expand the distribution function in terms of sums of scalar products of tensors formed from \( r \) and \( c \). These coefficients may or may not be functions of time depending on the system considered.

The distribution function is generally anisotropic in velocity space, independent of the presence of a magnetic field. The angular dependence of the phase-space distribution function in velocity space can be represented in terms of an expansion in spherical harmonics

\[ f(r, c, t) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} f_m^{(l)}(r, c, t) Y_m^{(l)}(\hat{c}) . \] (2.44)

where \( Y_m^{(l)}(\hat{c}) \) are spherical harmonics and \( \hat{c} \) denotes the angles of \( c \). Note that no restrictions are placed on the number of spherical harmonics nor is any particular form for the time-dependence of the expansion coefficients assumed. This expansion has to do with the velocity space and applies for either hydrodynamic or non-hydrodynamic conditions.

#### 2.4.2 Boltzmann equation decomposed in a spherical harmonics basis

The Boltzmann equation (1.1) describing the evolution of the phase-space distribution function \( f(r, c, t) \) of the charged particles for the time-dependent electric and magnetic fields can be written in the following form

\[ \frac{\partial f}{\partial t} + c \cdot \frac{\partial f}{\partial r} + \left[ a(t) + c \times \Omega(t) \right] \cdot \frac{\partial f}{\partial v} = -J(f, f_0) , \] (2.45)

where

\[ a(t) = \frac{q}{m} E(t) , \] (2.46)

is the acceleration due to a uniform time-dependent electric field and

\[ \Omega(t) = \frac{q}{m} B(t) , \] (2.47)

is the time-dependent cyclotron frequency in a uniform time-dependent magnetic field. Following the previous work of Ness (1993) we introduce the quantity

\[ c \times \Omega(t) = -\Omega(t) \cdot L , \] (2.48)
is reminiscent of the angular momentum operator in quantum mechanics. Hence the Boltzmann equation (2.45) has the following form

\[
\left( \partial_t + c \cdot \partial_r + a(t) \cdot \partial_c - \Omega(t) \cdot L \right) f(r, c, t) = -J(f, f_0)
\]  

Substitution of expansion (2.44) into (2.50), pre-multiplying on the left by the standard spherical harmonics \( \sum_{l'=-l'}^{l} <l l'| l' l' m>| c \cdot \nabla | l l' m > f_{m'}^{(l')} (r, c, t) \) and integrating over all angles \( \hat{c} \) yields the following system of coupled integro-differential equations for the standard tensorial expansion coefficients \( f_{m'}^{(l')} (r, c, t) \)

\[
\sum_{l'=0}^{\infty} \sum_{m'=-l'}^{l'} \langle l m| \partial_t + c \cdot \partial_r + a(t) \cdot \partial_c - \Omega(t) \cdot L | l' m' \rangle f_{m'}^{(l')} (r, c, t) = \sum_{l'=0}^{\infty} \sum_{m'=-l'}^{l'} \langle l m| J | l' m' \rangle f_{m'}^{(l')} (r, c, t)
\]

\[
= - \sum_{l'=0}^{\infty} \sum_{m'=-l'}^{l'} \langle l m| J | l' m' \rangle f_{m'}^{(l')} (r, c, t)
\]

Evaluating each matrix element partially using the Wigner-Eckart theorem (2.12) we have:

1. \[
\langle l m| \partial_t | l' m' \rangle f_{m'}^{(l')} (r, c, t) = \int Y_m^{(l)} (\hat{c}) \partial_t Y_{m'}^{(l')} (\hat{c}) d\hat{c} f_{m'}^{(l')} (r, c, t)
\]

\[
= \partial_t f_{m'}^{(l')} (r, c, t) \delta_{l l'} \delta_{m m'}
\]

i.e. diagonal in both the \( l \) and \( m \) indices (indicating the scalar nature of the operator).

2. \[
\langle l m| c \cdot \nabla | l' m' \rangle f_{m'}^{(l')} (r, c, t) = \int Y_m^{(l)} (\hat{c}) c \cdot \nabla Y_{m'}^{(l')} (\hat{c}) d\hat{c} f_{m'}^{(l')} (r, c, t)
\]

\[
= \sum_{\mu=-1}^{1} \int Y_m^{(l)} (\hat{c}) \mathbf{c}_\mu^{(l)} Y_{m'}^{(l')} (\hat{c}) d\hat{c} G^{(11)}_\mu f_{m'}^{(l')} (r, c, t)
\]

\[
= \sum_{\mu=-1}^{1} (l' m' 1 \mu | l m) \int l || \mathbf{c}_\mu^{(l)} || l' > G^{(11)}_\mu f_{m'}^{(l')} (r, c, t)
\]

where

\[
c \cdot \nabla = \sum_{\mu=-1}^{1} \mathbf{c}_\mu^{(l)} G^{(11)}_\mu
\]

3. \[
\langle l m| a(t) \cdot \frac{\partial}{\partial c} | l' m' \rangle f_{m'}^{(l')} (r, c, t) = \int Y_m^{(l)} (\hat{c}) a(t) \cdot \frac{\partial}{\partial c} Y_{m'}^{(l')} (\hat{c}) d\hat{c} f_{m'}^{(l')} (r, c, t)
\]

\[
= \sum_{\mu=-1}^{1} a^{(1)}_\mu (t) \int Y_m^{(l)} (\hat{c}) c_\mu^{(l)} Y_{m'}^{(l')} (\hat{c}) d\hat{c} f_{m'}^{(l')} (r, c, t)
\]

\[
= \sum_{\mu=-1}^{1} a^{(1)}_\mu (t) (l' m' 1 \mu | l m) \int l || c_\mu^{(l)} || l' > f_{m'}^{(l')} (r, c, t)
\]

53
If we define our co-ordinate system such that the electric field is parallel to the \( z \)-axis, then

\[
a^{(1)}_\mu(t) = -i a(t) \delta_{\mu 0}
\]  

(2.57)

and

\[
< lm | \mathbf{a}(t) \cdot \frac{\partial}{\partial \mathbf{c}} | l'm' > \ f_{m'}^{(l')} (r,c,t) = -ia(t)(l'm0|lm) < l||\partial_\mathbf{c}^{[1]}||l' > \ f_{m'}^{(l')} (r,c,t) \delta_{mm'}.
\]  

(2.58)

The explicit expressions for the reduced matrix elements in (2.54) and (2.58) are given by

\[
\begin{align*}
< lm | \Omega(t) \cdot \mathbf{L} | l'm' > \ f_{m'}^{(l')} (r,c,t) &= \int Y_m^{(l)}(\hat{e}) \Omega(t) \cdot \mathbf{L} Y_{m'}^{(l')} (\hat{e}) d\hat{e} f_{m'}^{(l')} (r,c,t) \\
&= \sum_{\mu = -1}^{1} \Omega^{[1]}_{\mu}(t) \int Y_m^{(l)}(\hat{e}) L_{\mu}^{[1]} Y_{m'}^{(l')} (\hat{e}) d\hat{e} f_{m'}^{(l')} (r,c,t) \\
&= -i \sum_{\mu = -1}^{1} \Omega^{[1]}_{\mu}(t)(l'm'1\mu|lm) < l||L^{[1]}||l' > \ f_{m'}^{(l')} (r,c,t)
\end{align*}
\]  

(2.59)

where

\[
< l||L^{[1]}||l' > = -\sqrt{l(l+1)} \delta_{ll'}
\]  

(2.60)

so that the magnetic field term is diagonal in the \( l \) index, independent of the configuration of \( \mathbf{E} \) and \( \mathbf{B} \).

Equation (2.61) implies that the collision matrix elements are diagonal in the \( l \) and \( m \) indices and independent of the latter. Notice that the reduced matrix element \( J^l \) is the scalar operator in the speed \( c \) space.

Hence, combining (2.53), (2.54), (2.58), (2.59) and (2.61) the system of equations (2.52) becomes

\[
\sum_{l' = 0}^{\infty} \sum_{m' = -l'}^{l'} \left\{ \partial_\mathbf{L}^{[1]} \delta_{mm'} + \sum_{\mu = -1}^{1} (l'm'1\mu|lm) < l||c^{[1]}||l' > G^{(11)}_{\mu}(t) \right\} \\
- ia(t) (l'm0|lm) < l||c^{[1]}||l' > \delta_{mm'} - \sum_{\mu = -1}^{1} \Omega^{[1]}_{\mu}(t)(l'm'1\mu|lm) < l||L^{[1]}||l' > \right\} f_{m'}^{(l')} (r,c,t)
\]  

\[
= -\sum_{l' = 0}^{\infty} \sum_{m' = -l'}^{l'} \left\{ J^l \delta_{ll'} \delta_{mm'} \right\} f_{m'}^{(l')} (r,c,t).
\]  

(2.62)

The explicit expressions for the reduced matrix elements in (2.54) and (2.58) are given by
Robson and Ness (1986):

\[
\langle l||c^{[1]}||l' \rangle = \begin{cases} 
  c \sqrt{\frac{l}{2l+1}} & \text{if } l' = l - 1, \\
  c \sqrt{\frac{l+1}{2l+1}} & \text{if } l' = l + 1, \\
  0 & \text{otherwise}.
\end{cases} \tag{2.63}
\]

\[
\langle l||\partial_{E}^{[1]}||l' \rangle = \begin{cases} 
  \sqrt{\frac{l}{2l+1}} \left[ \frac{d}{dc} - \frac{l-1}{c} \right] & \text{if } l' = l - 1, \\
  \sqrt{\frac{l+1}{2l+1}} \left[ \frac{d}{dc} + \frac{l+2}{c} \right] & \text{if } l' = l + 1, \\
  0 & \text{otherwise}.
\end{cases} \tag{2.64}
\]

This system of differential equations represents the most general form having no inbuilt assumptions on the space- and time-dependence of the phase-space distribution function. It represents the starting point for any multi-term solution of the Boltzmann equation. In what follows we will consider what form these equations will take in two limiting cases: (i) time-dependent hydrodynamic regime; and (ii) steady-state non-hydrodynamic regime.

### 2.5 Time-dependent hydrodynamic regime

#### 2.5.1 The density gradient expansion in the time-dependent hydrodynamic regime

We now consider a time-dependent hydrodynamic description of the swarm, in which the spatial dependence of the distribution (and hence the standard tensorial coefficients \( f_{m}^{(l)}(r, c, t) \)) is carried entirely by the number density and its spatial derivatives. In the presence of both electric and magnetic fields, there are three independent directions in any swarm experiment\(^1\). These directions are determined by the electric field vector \( E(t) = (E(t) \hat{E}_0) \), the magnetic field vector \( B(t) = (B(t) \hat{B}_0) \), and spatial gradients \( \nabla n \). It is thus possible to form tensors of any rank from these three vectors (either individually or by coupling them together). The most general expansion of \( f_{m}^{(l)}(r, c, t) \) (and any quantity which is a function of \( r \)) is a sum over all the possible tensors of rank \( l \) and component \( m \) resulting from couplings of \( E(t) \), \( B(t) \) and \( \nabla n \). In irreducible tensor form we thus have

\[
f_{m}^{(l)}(r, c, t) = \sum_{s=0}^{\infty} \sum_{\lambda=0}^{\lambda} \sum_{\lambda'=0}^{\lambda} \sum_{\lambda''=0}^{\lambda} \sum_{\lambda'''=0}^{\lambda} \hat{f}(l|s\lambda \lambda' \lambda'' \lambda'''|; c, t) \left[ \begin{array}{c} Y^{(\lambda''')} (\hat{E}_0), Y^{(\lambda'')} (\hat{B}_0) \end{array} \right]^{(l)}_{m} n(r, t),
\]

where \( \hat{f}(l|s\lambda \lambda' \lambda'' \lambda'''|; c, t) \) are scalar coefficients which vanish unless

\[
l + \lambda + \lambda'' + \lambda''' = \text{even},
\]

a result of parity consideration and independent of the configuration of \( E \) and \( B \). The order of the coupling of the tensors in (2.65) is arbitrary. If the electric field is oriented along the z axis,

\(^{1}\)To our knowledge, the swarms experiments under conditions of time-dependent electric and magnetic fields are not developed.
then from (2.1) we have

$$Y^{(\lambda''')}_{\mu'''}(\hat{E}_0) = (-i)^{\lambda'''} \left( \frac{2\lambda'''}{4\pi} + 1 \right)^{1/2} \delta_{\mu'0} \ .$$ (2.67)

Employing the tensor coupling rule (2.4) in (2.65) and using the expression (2.67) we find

$$f_m^{(l)}(r, c, t) = \sum_{s=0}^{\infty} \sum_{\lambda=0}^{\infty} \sum_{\mu=0}^{\infty} f(lm|s\lambda\mu; c, t)G_{\mu}^{(s)}(s\lambda)(r, t) \ ,$$ (2.68)

where

$$\bar{f}(lm|s\lambda\mu; c, t) = \sum_{s'=0}^{\infty} \sum_{\lambda'=0}^{\infty} \sum_{\mu'=0}^{\infty} (-i)^{\lambda'''} \left( \frac{2\lambda'''}{4\pi} + 1 \right)^{1/2} (\lambda'm - \mu\lambda\mu|lm)

(\lambda''0\lambda''m - \mu|\lambda'm - \mu)f(l|s\lambda\lambda''\lambda''''; c, t)Y^{\lambda'''}_{\mu'''}(\hat{B}_0) \ .$$ (2.69)

Certain important properties of the expansion coefficients in (2.68) are of considerable interest. These properties are independent of the temporal form of electric and magnetic fields and include the following:

1. \(f(lm|s\lambda\mu; c, t) = 0 \) if \( |m| > \min\{\lambda, l\} \) (2.70)

This follows from the restrictions imposed on the Clebsch-Gordan coefficient in (2.69).

2. \(f(lm|s\lambda\mu; c, t) = 0 \) if \(|\mu| > \lambda \) or \( \lambda > s \) (2.71)

This symmetry property results from the restrictions imposed on the gradient tensor and the Clebsch-Gordan coefficient in (2.69).

3. \(f^*(lm|s\lambda\mu; c, t) = (-1)^{l+m+\lambda+\mu} f(l - m|s\lambda - \mu; c, t) \) (2.72)

This property follows by enforcing reality on \(f(r, c, t)\) and taking the complex conjugate of (2.68). In addition, the following symmetry properties of the moments can be shown to exist (White et al.) (1999):

$$f(lm|s\lambda\mu; -E, B) = (-1)^{l+\lambda} f(lm|s\lambda\mu; E, B) \ ,$$ (2.73)

$$f(lm|s\lambda\mu; E, -B_y, B_z) = (-1)^{m+\mu} f(lm|s\lambda\mu; E, B) \ ,$$ (2.74)

$$f(lm|s\lambda\mu; E, B_y, -B_z) = (-1)^{m+\mu} f(l - m|s\lambda - \mu; E, B) \ ,$$ (2.75)

$$f(lm|s\lambda\mu; E, -B) = f(l - m|s\lambda - \mu; E, B) \ .$$ (2.76)

In summary, combining expressions (2.44) and (2.68), the expansion of the spatial and (angular part of the) velocity dependence of the phase-space distribution function in terms of spherical tensors is given by

$$f(r, c, t) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \sum_{s=0}^{\infty} \sum_{\lambda=0}^{\infty} \sum_{\mu=0}^{\infty} f(lm|s\lambda\mu; c, t)Y_m^{(l)}(\hat{c})G_{\mu}^{(s)}(s\lambda)(r, t) \ .$$ (2.77)
If we take terms up to \( s = 2 \) (the second order density gradient expansion), the phase-space distribution function may be written in the form

\[
f(r, c, t) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} f(lm|000; c, t)\hat{Y}_m^l(\hat{c})n(r, t) + \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \sum_{\mu=-1}^{1} f(lm|11\mu; c, t)\hat{Y}_m^l(\hat{c})G_{\mu}^{(1)}(r, t) + \\
\sum_{l=0}^{1} \sum_{m=-l}^{l} f(lm|200; c, t)\hat{Y}_m^l(\hat{c})G_{\mu}^{(20)}(r, t) + \\
\sum_{l=0}^{1} \sum_{m=-l}^{l} \sum_{\mu=-2}^{2} f(lm|22\mu; c, t)\hat{Y}_m^l(\hat{c})G_{\mu}^{(22)}(r, t) .
\]  

(2.78)

From (2.78), we observe that even for the spatially homogeneous case, an expansion in terms of Legendre polynomials is inadequate beyond the two-term limit (Ness, 1993). In the special case of the two-term approximation where the sums are truncated at \( l = 1 \), if the polar axis is oriented along the vector \( f_m^{(l)} \), the Legendre polynomials may be used. Another special case is associated with the parallel configuration of the fields. In such a case there exists a single axis of symmetry and terms to first order in the spatial gradients in (2.78) can be reduced to expansions in terms of Legendre polynomials, as in the case when only an electric field is present. Note that even for swarms in electric field only, transverse spatial gradients destroy rotational symmetry in velocity space and Legendre polynomial expansion is thus invalid for spatially inhomogeneous conditions. Therefore, a multi-term representation of the distribution function in electric and magnetic fields requires a full spherical harmonic decomposition.

### 2.5.2 Hierarchy of kinetic equations

We substitute (2.68) into the spherical harmonic representation of the Boltzmann equation (2.62) and equate the coefficients of \( G_{\mu}^{(s\lambda)} \). The result is a hierarchy of coupled first order integro-differential equations for the scalar expansion coefficients \( f(lm|s\lambda\mu; c, t) \). We consider each term of (2.62) separately.

\[
\partial_t f_m^{(l)}(r, c, t) = \partial_t \left[ \sum_{s'=0}^{\infty} \sum_{\lambda'=0}^{\lambda'} \sum_{\mu'=-\lambda'}^{\lambda'} f(lm|s'\lambda'\mu'; c, t)G_{\mu'}^{(s'\lambda')} n(r, t) \right]
\]  

\[
= \sum_{s'=0}^{\infty} \sum_{\lambda'=0}^{\lambda'} \sum_{\mu'=-\lambda'}^{\lambda'} \left[ \partial_t f(lm|s'\lambda'\mu'; c, t)G_{\mu'}^{(s'\lambda')} n(r, t) + f(lm|s'\lambda'\mu'; c, t)G_{\mu'}^{(s'\lambda')} \partial_t n(r, t) \right] .
\]  

(2.79)

Since \( \partial_t n(r, t) \) is a scalar, we can express it in this way (Robson and Ness, 1986)

\[
\partial_t n(r, t) = \sum_{s''=0}^{\infty} \sum_{\lambda''=0}^{\lambda''} \sum_{\mu''=-\lambda''}^{\lambda''} \omega(s''\lambda''\mu'', t)G_{\mu''}^{(s''\lambda'')} n(r, t) ,
\]  

(2.80)
where the scalar coefficients $\omega(s''\lambda''\mu'', t)$ are dependent on time. Applying the inverse coupling rule (2.6) we have

$$G^{(s'\lambda')}_{\mu'} G^{(s''\lambda'')}_{\mu''} = \sum_{\lambda=0}^{s'} \sum_{\mu=-\lambda}^{\lambda} (\lambda' \mu' \lambda'' \mu'' | \bar{\lambda} \bar{\mu}) G^{(s'+s'', \lambda)}_{\lambda},$$  \hspace{1cm} \text{(2.81)}

where $(s' + s'' \leq 2)$. Using (2.80) and (2.81) the expression (2.79) becomes

$$\partial_t f_m^{(l)}(s, \mu, c, t) = \sum_{s'=0}^{\infty} \sum_{\lambda'=0}^{\lambda'} \sum_{\mu'=-\lambda'}^{\lambda'} \left[ \partial_t f(lm|s'\lambda'\mu'; c, t) G^{(s'\lambda')}_{\mu'} n(r, t) \right] + \sum_{s''=0}^{\infty} \sum_{\lambda''=0}^{\lambda''} \sum_{\mu''=-\lambda''}^{\lambda''} f(lm|s'\lambda'\mu'; c, t) \omega(s''\lambda''\mu''; t) (\lambda' \mu' \lambda'' \mu'' | \bar{\lambda} \bar{\mu}) G^{(s'+s'', \lambda)}_{\lambda} n(r, t) \right].$$  \hspace{1cm} \text{(2.82)}

Therefore, the coefficient of $G^{(s\lambda)}_{\mu} n(r, t)$ appearing in (2.82) is given by

$$\partial_t f(lm|s\lambda\mu; c, t) + \sum_{s_1=0}^{s} \sum_{\lambda_1=0}^{\lambda} \sum_{\mu_1=-\lambda_1}^{\lambda_1} \sum_{s_2=0}^{s-s_1} \sum_{\lambda_2=0}^{\lambda_2} \sum_{\mu_2=-\lambda_2}^{\lambda_2} (\lambda_1 \mu_1 \lambda_2 \mu_2 | \lambda \mu) \omega(s - s_1 \lambda_2 \mu_2; t) f(lm|s_1 \lambda_1 \mu_1; c, t).$$  \hspace{1cm} \text{(2.83)}

From (2.6) we have

$$G^{(11)}_{\mu} G^{(s_1 \lambda_1)}_{\mu_1} = \sum_{s_2=0}^{s_1+1} \sum_{\lambda_2=-\lambda_2}^{\lambda_2} (1 \mu_1 \lambda_1 | \lambda_2 \mu_2) G^{(s_1+1 \lambda_2)}_{\mu_2},$$  \hspace{1cm} \text{(2.85)}

Therefore, the coefficient of $G^{(s\lambda)}_{\mu}$ is given by

$$\sum_{l'=0}^{\infty} \sum_{m'=0}^{l'} \sum_{\lambda'_1=0}^{\lambda_1} \sum_{\mu'_1=-\lambda_1}^{\lambda_1} \sum_{l=0}^{l'} \sum_{m=0}^{l} \sum_{\lambda_2=0}^{\lambda} \sum_{\mu_2=-\lambda}^{\lambda} (l'm'\mu_1|lm)(1 \mu_1 \lambda_1 | \lambda_2 \mu_2) < l||c|| |l'| > f(l'm'|s - 1 \lambda_1 \mu_1; c, t).$$  \hspace{1cm} \text{(2.86)}

From (2.6) we have

$$\sum_{l'=0}^{\infty} \sum_{m'=0}^{l'} \sum_{\lambda'_1=0}^{\lambda_1} \sum_{\mu'_1=-\lambda_1}^{\lambda_1} \sum_{l=0}^{l'} \sum_{m=0}^{l} \sum_{\lambda_2=0}^{\lambda} \sum_{\mu_2=-\lambda}^{\lambda} (l'm'\mu_1|lm)(1 \mu_1 \lambda_1 | \lambda_2 \mu_2) < l||c|| |l'| > f(l'm'|s - 1 \lambda_1 \mu_1; c, t).$$  \hspace{1cm} \text{(2.86)}

Therefore, the coefficient of $G^{(s\lambda)}_{\mu}$ is given by

$$\sum_{l'=0}^{\infty} \sum_{m'=0}^{l'} \sum_{\lambda'_1=0}^{\lambda_1} \sum_{\mu'_1=-\lambda_1}^{\lambda_1} \sum_{l=0}^{l'} \sum_{m=0}^{l} \sum_{\lambda_2=0}^{\lambda} \sum_{\mu_2=-\lambda}^{\lambda} (l'm'\mu_1|lm)(1 \mu_1 \lambda_1 | \lambda_2 \mu_2) < l||c|| |l'| > f(l'm'|s - 1 \lambda_1 \mu_1; c, t).$$  \hspace{1cm} \text{(2.86)}
The coefficient of $G^{(s\lambda)}(r, t)$ is given by

$$
\sum_{l'=0}^{\infty} -ia(t)(l'm10|lm) < l||\varphi_c^{[1]}||l' > f(l'm|s\lambda\mu; c, t) .
$$

(2.88)

$$
\sum_{l'=0}^{\infty} \sum_{l''=l'}^{1} -\Omega^{[1]}_{\mu}(t)(l'm'1\mu|lm) < l||L^{[1]}||l' > f_{m'}(r, c, t)
$$

(4)

$$
= \sum_{l'=0}^{\infty} \sum_{l''=l'}^{1} \sum_{s'=0}^{1} \sum_{\lambda'}^{1} -\Omega^{[1]}_{\mu}(t)(l'm'1\mu|lm) < l||L^{[1]}||l' > f(l'm'|s'\lambda'\mu'; c, t)G^{(s'\lambda')}_{\mu'}(r, t) .
$$

(2.89)

Hence the coefficient of $G^{(s\lambda)}(r, t)$ is

$$
\sum_{l'=0}^{\infty} \sum_{l''=l'}^{1} -\Omega^{[1]}_{\mu}(t)(l'm'1\mu|lm) < l||L^{[1]}||l' > f(l'm'|s\lambda\mu; c, t) .
$$

(2.90)

$$
\sum_{l'=0}^{\infty} \sum_{l''=l'}^{1} \{ - J^{l'} f_{m'}(r, c, t) \delta_{mm'} \}
$$

(5)

$$
- \sum_{l'=0}^{\infty} \sum_{l''=l'}^{1} \sum_{s'=0}^{1} \sum_{\lambda'}^{1} J^{l'} \delta_{m'm'} f(l'm'|s'\lambda'\mu'; c, t)G^{(s'\lambda')}_{\mu'}(r, t) ,
$$

(2.91)

and the coefficient of $G^{(s\lambda)}(r, t)$ is

$$
-J^{l} f(lm|s\lambda\mu; c, t) .
$$

(2.92)

On substitution of (2.82), (2.85), (2.86), (2.89) and (2.91) into (2.62) and equating coefficients $G^{(s\lambda)}(r, t)$ yields from (2.83), (2.86), (2.88), (2.90) and (2.92) the following hierarchy of coupled operator equations (time-dependent kinetic equations) up to and including the second order density gradient

$$
[\partial_t + \omega(000; t) + J^{l}] f(lm|s\lambda\mu; c, t) - ia(t) \sum_{l'=0}^{\infty} (l'm10|lm) < l||\varphi_c^{[1]}||l' > f(l'm|s\lambda\mu; c, t)
$$

$$
- \sum_{l'=0}^{\infty} \sum_{l''=l'}^{1} \sum_{s'=0}^{1} \sum_{\lambda'}^{1} \Omega^{[1]}_{\mu}(t)(l'm'1\mu|lm) < l||L^{[1]}||l' > f(l'm'|s\lambda\mu; c, t) = X(lm|s\lambda\mu; c, t) ,
$$

(2.93)

where

$$
X(lm|s\lambda\mu; c, t) = - \sum_{s} \sum_{s_1} \sum_{\lambda_1} \sum_{s-s_1} \sum_{\lambda_2} (\lambda_1\mu_1\lambda_2\mu_2|\lambda\mu)(1 - \delta_{s_1s}\delta_{\lambda_20}\delta_{\mu_20})
$$

$$
\omega(s - s_1\lambda_2\mu_2; t) f(lm|s_1\lambda_1\mu_1; c, t)
$$

$$
\sum_{l'=0}^{\infty} \sum_{l''=l'}^{1} \sum_{s-1}^{1} \sum_{\lambda_1} (l'm'1\mu|lm)(1\mu_1\lambda_1\lambda_1|\lambda\mu) < l||c^{[1]}||l' > f(l'm'|s - 1\lambda_1\mu_1; c, t) .
$$

(2.94)
In order to find the expansion coefficients $\omega(s\lambda\mu; t)$ we apply the following restriction

$$\sqrt{4\pi} \int_{0}^{\infty} f(00|s\lambda\mu; c, t)c^{2}dc = \delta_{s0}\delta_{\lambda0}\delta_{\mu0},$$  

(2.95)

which can be obtained through normalization considerations. Another useful property is given by

$$\int_{0}^{\infty} <\omega_{C}|1 > \phi(c)c^{2}dc = 0,$$  

(2.96)

if $\phi(c)$ is any well-behaved function on the interval $(0, \infty)$.

Multiplying the $l = 0$ and $m = 0$ members of (2.93) by $c^{2}$ and integrating over all speeds, we have through the use of (2.95) and (2.96) the following expression for the expansion coefficient appearing in (2.80)

$$\omega(s\lambda\mu; t) = \sqrt{4\pi/3} \int_{0}^{\infty} \sum_{m=-l}^{l} (-1)^{l}(1\bar{\mu}\lambda_{1}\mu - \mu|\lambda\mu)cf(1 - \bar{\mu}|s - 1\lambda_{1}\mu - \bar{\mu}; c, t)c^{2}dc$$

$$- \sqrt{4\pi} \int_{0}^{\infty} n_{0}J_{R}^{0}f(00|s\lambda\mu; c, t)c^{2}dc,$$  

(2.97)

where $J_{R}$ denotes the reactive part of the collision operator.

### 2.5.3 Change in the form of hierarchy equations through inclusion of the time-dependent magnetic field

There are some important differences in the hierarchy members which result when the explicit time dependence of the expansion coefficients $f(lm|\lambda\mu; c, t)$ and $\omega(s\lambda\mu; t)$ are retained as compared with the steady-state dc treatment of Ness (1993; 1994) and ac treatment of White (1996) and White et al. (1995; 1998; 1999b). As mentioned previously, in this thesis we employ a coordinate system in which the $z$ axis is defined by the electric field vector while the magnetic field vector lies in the $y-z$ plane making an angle $\psi$ with respect to electric field vector. For this specific configuration, the hierarchy of coupled differential equations (2.93) may be written as:

$$\left[\partial_{t} + \omega(000; t) + J^{l}\right]f(lm|s\lambda\mu; c, t) = ia(t)\sum_{l'=0}^{\infty} (l'm10|lm) <l||\omega_{C}||l'> f(l'm|s\lambda\mu; c, t)$$

$$+ \sum_{l'=0}^{\infty} \sum_{m'=l'}^{l} \frac{q}{m} B(t) \left\{ \frac{\sin \psi}{2} \left[ \sqrt{(l+m)(l-m+1)}\delta_{m'-m-1} - \sqrt{(l-m)(l+m+1)}\delta_{m'+m+1} \right. \right.$$

$$\left. + im\cos \psi\delta_{m'm} \right\} \delta_{l'l}f(l'm'|s\lambda\mu; c, t) = X(lm|s\lambda\mu; c, t).$$  

(2.98)

Equation (2.98) constitutes a hierarchy of coupled 2-dimensional integro-partial-differential equations for the expansion coefficients $f(lm|s\lambda\mu; c, t)$. Each member in the hierarchy is defined uniquely by the triplet $(s, \lambda, \mu)$. The $s$-index defines the 'level' of equations. The 'sets' of each level are characterized by the $\lambda$ index. Each set has $2\lambda + 1$ members according the allowed values of the $\mu$-index $(-\lambda \leq \mu \leq \lambda)$. Each member of the hierarchy represents an infinite set of coupled 2-dimensional-integro-differential equations as dictated by the $l$-index. For a given
level (or $s$-value), we observe from (2.98) that the members of that level (defined by $\lambda$ and $\mu$) do not couple with other members in that level. These members are coupled only with members of lower levels. Thus in solving the hierarchy, solution of the lower level is required before proceeding to the next level.

The first member of hierarchy (2.98) (defined by $s = \lambda = \mu = 0$) is the spatially homogeneous member. It represents the homogeneous counterpart to those discussed above for $s \geq 1$. From (2.97) we see that the $\omega(s\lambda\mu; t)$ appearing on the rhs of (2.98) is unknown. Thus, if non-conservative collisions are operative, then (2.97) and (2.98) represent a non-linear system of equations which must be solved in some self-consistent manner for $f(lm|\lambda\mu; c, t)$ and $\omega(s\lambda\mu; t)$. We employ similar technique as for the ac electric field only case (White (1996); White et al. (1995; 1998; 1999b)). In the absence of non-conservative collisions, $\omega(s\lambda\mu; t) = 0$ and the spatially homogeneous member $((s, \lambda, \mu) = (0, 0, 0))$ is directly solvable. The members defined by $s \geq 1$ represent an inhomogeneous operator equation and as remarked previously, all terms appearing on the rhs of (2.98) are determined from lower level moments.

One should note carefully the differences between the hierarchy members appearing in this thesis and those specified by Ness (1993; 1994) for a dc electric and magnetic field configuration and those specified by White (1996) within an ac electric field only treatment. With respect to dc treatment of Ness (1993; 1994), most notably difference is the explicit addition of the partial time derivative operator to the coefficient operator matrix. It is evident from (2.98) that the time-derivative operator is diagonal in both $l$ and $m$ indices. Therefore, in contrast to a dc treatment of Ness (1993; 1994) where the each member of the hierarchy represent the 1-dimensional integro-differential equation, for ac electric and magnetic fields crossed at arbitrary angle considered in this thesis, each member of the hierarchy (2.98) represent the 2-dimensional integro-partial-differential equation. Another difference with respect to a dc treatment is associated with the spatially homogeneous member of the hierarchy. As remarked by White (1996) and White et al. (1999b), in the presence of non-conservative processes and a time-varying field (no matter how slight), this member is no longer a true eigenvalue problem. Hence the implications of the physical interpretation of the spectrum of eigenvalues in the steady-state problem (Robson and Ness (1986); Ness (1993; 1994)) do not appear to carry over to the periodic steady-state.

With regard to the differences with respect to an ac electric field only treatment of White (1996) and White et al. (1998; 1999b), we note the explicit addition of magnetic field term to the coefficient matrix. The reduced matrix elements of the normal component of the magnetic field are diagonal in both the $l$ and $m$ indices while the parallel component is diagonal in $l$ index but sub-diagonal ($m = m' - 1$) and super-diagonal ($m = m' + 1$) in the $m$ index. The application of a magnetic field does not change the structure of the electric field term. The electric field term contains the reduced matrix elements of the velocity differential operator and it is easy to see from (2.64) that it is both sub-diagonal and super-diagonal in the $l$-indices and diagonal in the $m$-index.
2.5.4 Transport coefficients and transport properties in the time-dependent hydrodynamic regime

2.5.4.1 Transport coefficients

As discussed previously, the bulk transport coefficients in the time-dependent hydrodynamic regime are defined as the coefficients of the number density and its spatial derivatives in the time-dependent diffusion equation (2.25). Using the explicit expressions for $G^{(s)}_{\mu}$ (from Table 2.1) in the spherical form of the continuity equation (2.80), the relationship between the spherical quantities $\omega(s_{\lambda\mu}; t)$ and their Cartesian counterparts in (2.25) can be established. The explicit form of the transport coefficients in terms of the calculated moments $f(lm|s_{\lambda\mu}; c, t)$ are given by:

(1) The loss rate:

$$\alpha(t) = -\omega(000; t) = -\sqrt{4\pi} \int_0^\infty n_0 J^0_R f(0000; c, t) c^2 dc . \quad (2.99)$$

(2) The bulk drift velocity components:

$$W_x(t) = -\frac{i}{\sqrt{2}} \left[ \omega(111; t) - \omega(11 - 1; t) \right]$$

$$= \sqrt{\frac{8\pi}{3}} \int_0^\infty c^3 \text{Im} \left\{ f(1100; c, t) \right\} dc - \sqrt{8\pi} \int_0^\infty n_0 J^0_R \text{Im} \left\{ f(0011; c, t) \right\} c^2 dc , \quad (2.100)$$

$$W_y(t) = -\frac{1}{\sqrt{2}} \left[ \omega(111; t) + \omega(11 - 1; t) \right]$$

$$= \sqrt{\frac{8\pi}{3}} \int_0^\infty c^3 \text{Re} \left\{ f(1100; c, t) \right\} dc + \sqrt{8\pi} \int_0^\infty n_0 J^0_R \text{Re} \left\{ f(0011; c, t) \right\} c^2 dc , \quad (2.101)$$

$$W_z(t) = i\omega(110; t)$$

$$= -\sqrt{\frac{4\pi}{3}} \int_0^\infty c^3 \text{Im} \left\{ f(1000; c, t) \right\} dc + \sqrt{4\pi} \int_0^\infty n_0 J^0_R \text{Im} \left\{ f(0011; c, t) \right\} c^2 dc . \quad (2.102)$$

(3) The bulk diagonal diffusion tensor components:

$$D_{xx}(t) = \frac{1}{\sqrt{3}} \omega(200; t) + \frac{1}{\sqrt{6}} \omega(220; t) - \frac{1}{2} [\omega(222; t) + \omega(22 - 2; t)]$$

$$= -\sqrt{\frac{4\pi}{3}} \int_0^\infty c^3 \left[ \text{Re} \left\{ f(1111; c, t) \right\} - \text{Re} \left\{ f(1 - 11; c, t) \right\} \right] dc$$

$$- \sqrt{\frac{4\pi}{3}} \int_0^\infty n_0 J^0_R \left[ f(0020; c, t) + \frac{1}{\sqrt{2}} f(0022; c, t) - \sqrt{3} \text{Re} \left\{ f(0022; c, t) \right\} \right] , \quad (2.103)$$

$$D_{yy}(t) = \frac{1}{\sqrt{3}} \omega(200; t) + \frac{1}{\sqrt{6}} \omega(220; t) + \frac{1}{2} [\omega(222; t) + \omega(22 - 2; t)]$$

$$= -\sqrt{\frac{4\pi}{3}} \int_0^\infty c^3 \left[ \text{Re} \left\{ f(1111; c, t) \right\} + \text{Re} \left\{ f(1 - 11; c, t) \right\} \right] dc$$

$$- \sqrt{\frac{4\pi}{3}} \int_0^\infty n_0 J^0_R \left[ f(0020; c, t) + \frac{1}{\sqrt{2}} f(0022; c, t) + \sqrt{3} \text{Re} \left\{ f(0022; c, t) \right\} \right] , \quad (2.104)$$
The bulk off-diagonal elements of the diffusion tensor:

\[ D_{zz}(t) = \frac{1}{\sqrt{3}} \omega(200; t) - \sqrt{\frac{2}{3}} \omega(220; t) \]

\[ = -\sqrt{\frac{4\pi}{3}} \int_0^\infty c^3 f(10|110; c, t) - \sqrt{\frac{4\pi}{3}} \int_0^\infty n_0 J_R^0 \left[ f(00|200; c, t) - \sqrt{2} f(00|220; c, t) \right] . \]  

(2.105)

(4) The bulk off-diagonal elements of the diffusion tensor:

\[ D_1(t) = D_{xy}(t) + D_{yx}(t) = i[\omega(222; t) - \omega(22 - 2; t)] \]

\[ = \sqrt{\frac{16\pi}{3}} \int_0^\infty c^3 \text{Im} \left\{ f(1 - 1|111; c, t) \right\} dc + \sqrt{16\pi} \int_0^\infty n_0 J_R^0 \text{Im} \left\{ f(00|222; c, t) \right\} c^2 dc , \]  

(2.106)

\[ D_2(t) = D_{xz}(t) + D_{zx}(t) = [\omega(221; t) - \omega(22 - 1; t)] \]

\[ = \sqrt{\frac{8\pi}{3}} \int_0^\infty c^3 \left[ \text{Re} \left\{ f(10|111; c, t) \right\} - \text{Re} \left\{ f(1 - 1|110; c, t) \right\} \right] dc 

- \sqrt{16\pi} \int_0^\infty n_0 J_R^0 \text{Re} \left\{ f(00|221; c, t) \right\} c^2 dc , \]  

(2.107)

\[ D_3(t) = D_{yz}(t) + D_{zy}(t) = -i[\omega(221; t) - \omega(22 - 1; t)] \]

\[ = \sqrt{\frac{8\pi}{3}} \int_0^\infty c^3 \left[ \text{Im} \left\{ f(10|111; c, t) \right\} - \text{Im} \left\{ f(1 - 1|110; c, t) \right\} \right] dc 

- \sqrt{16\pi} \int_0^\infty n_0 J_R^0 \text{Im} \left\{ f(00|221; c, t) \right\} c^2 dc , \]  

(2.108)

The corresponding flux transport coefficients defined in (2.29) and (2.30) are given by:

- The flux components of the drift velocity:

\[ W_x^{(s)}(t) = \sqrt{\frac{8\pi}{3}} \int_0^\infty c^3 \text{Im} \left\{ f(11|000; c, t) \right\} dc , \]  

(2.109)

\[ W_y^{(s)}(t) = \sqrt{\frac{8\pi}{3}} \int_0^\infty c^3 \text{Re} \left\{ f(1 - 1|000; c, t) \right\} dc , \]  

(2.110)

\[ W_z^{(s)}(t) = \sqrt{\frac{4\pi}{3}} \int_0^\infty c^3 \text{Im} \left\{ f(10|000; c, t) \right\} dc . \]  

(2.111)

- The flux diagonal diffusion tensor components:

\[ D_{xx}^{(s)}(t) = -\sqrt{\frac{4\pi}{3}} \int_0^\infty c^3 \left[ \text{Re} \left\{ f(11|111; c, t) \right\} - \text{Re} \left\{ f(1 - 1|111; c, t) \right\} \right] dc , \]  

(2.112)

\[ D_{yy}^{(s)}(t) = -\sqrt{\frac{4\pi}{3}} \int_0^\infty c^3 \left[ \text{Re} \left\{ f(11|111; c, t) \right\} + \text{Re} \left\{ f(1 - 1|111; c, t) \right\} \right] dc , \]  

(2.113)

\[ D_{zz}^{(s)}(t) = -\sqrt{\frac{4\pi}{3}} \int_0^\infty c^3 f(10|110; c) dc . \]  

(2.114)

- The flux off-diagonal elements of the diffusion tensor:

\[ D_1^{(s)}(t) = \sqrt{\frac{16\pi}{3}} \int_0^\infty c^3 \left\{ \text{Im} \left\{ f(1 - 1|111; c, t) \right\} \right\} dc , \]  

(2.115)

\[ D_2^{(s)}(t) = \sqrt{\frac{8\pi}{3}} \int_0^\infty c^3 \left[ \text{Re} \left\{ f(1 - 1|111; c, t) \right\} - \text{Re} \left\{ f(1 - 1|110; c, t) \right\} \right] dc , \]  

(2.116)

\[ D_3^{(s)}(t) = \sqrt{\frac{8\pi}{3}} \int_0^\infty c^3 \left\{ \text{Im} \left\{ f(10|111; c, t) \right\} - \text{Im} \left\{ f(1 - 1|110; c, t) \right\} \right\} dc . \]  

(2.117)
Expressions for the off-diagonal elements of the diffusion tensor are not directly obtainable from the diffusion equation, but rather must be obtained from the flux-gradient relation (2.22) (White et al., 1999a). These quantities are given by:

\[
D_{xy}(t) = \sqrt{\frac{4\pi}{3}} \int_0^\infty c^3 \left[ \operatorname{Im} \left\{ f(1 - 1|111; c, t) \right\} - \operatorname{Im} \left\{ f(11|111; c, t) \right\} \right] dc , \quad (2.118)
\]

\[
D_{xz}(t) = \sqrt{\frac{8\pi}{3}} \int_0^\infty c^3 \operatorname{Re} \left\{ f(11|110; c, t) \right\} dc , \quad (2.119)
\]

\[
D_{yz}(t) = \sqrt{\frac{4\pi}{3}} \int_0^\infty c^3 \left[ \operatorname{Im} \left\{ f(11|111; c, t) \right\} - \operatorname{Im} \left\{ f(1 - 1|111; c, t) \right\} \right] dc , \quad (2.120)
\]

\[
D_{yz}(t) = -\sqrt{\frac{8\pi}{3}} \int_0^\infty c^3 \operatorname{Im} \left\{ f(11|110; c, t) \right\} dc , \quad (2.121)
\]

\[
D_{xz}(t) = \sqrt{\frac{8\pi}{3}} \int_0^\infty c^3 \operatorname{Re} \left\{ f(10|111; c, t) \right\} dc , \quad (2.122)
\]

\[
D_{xy}(t) = \sqrt{\frac{8\pi}{3}} \int_0^\infty c^3 \operatorname{Im} \left\{ f(10|111; c, t) \right\} dc . \quad (2.123)
\]

### 2.5.4.2 Transport properties

The average energy \( \epsilon(r, t) \) plays an important role in understanding various phenomena associated with drift and diffusion coefficients. In particular, we utilize the following two important transport parameters: (i) the spatially homogeneous mean energy \( \bar{\epsilon}(t) \); and (ii) gradient energy parameter \( \gamma(t) \). The latter was introduced by White et al. (1995). These quantities are defined through a density gradient expansion of the mean energy:

\[
\epsilon(r, t) = \frac{1}{n(r, t)} \int \frac{1}{2} mc^2 f(c, r, t) dc = \bar{\epsilon}(t) + \gamma(t) \cdot \nabla \frac{n}{n} + \zeta(t) : \nabla \nabla \frac{n}{n} + \ldots , \quad (2.124)
\]

where \( \zeta(t) \) is the diffusive energy tensor. Substitution of (2.77) into (2.124) yields the following equation for the average energy

\[
\epsilon(r, t) = \sqrt{4\pi} \int_0^\infty \frac{1}{2} mc^2 f(00|000; c, t) c^2 dc \\
+ \sqrt{\frac{4\pi}{n(r, t)}} \int_0^\infty \frac{1}{2} mc^2 \sum_{s=0}^{\infty} \sum_{\lambda=0}^{\infty} \sum_{\mu=0}^{\lambda} \int f(00|s\lambda\mu; c, t)(1 - \delta_{s0}\delta_{\lambda0}\delta_{\mu0}) c^2 dc G_{\mu}^{(s\lambda)} n(r, t) . \quad (2.125)
\]

Comparing (2.124) and (2.125), we identify the spatially homogeneous mean energy

\[
\bar{\epsilon}(t) = \sqrt{4\pi} \int_0^\infty \frac{1}{2} mc^2 f(00|000; c, t) c^2 dc . \quad (2.126)
\]

Truncation of (2.125) at \( s = 1 \) yields the components of the gradient energy vector:

\[
\gamma_x(t) = -\sqrt{4\pi} \int_0^\infty \frac{1}{2} mc^2 \left[ \sqrt{2} \operatorname{Im} \left\{ f(00|111; c, t) \right\} \right] c^2 dc , \quad (2.127)
\]

\[
\gamma_y(t) = \sqrt{4\pi} \int_0^\infty \frac{1}{2} mc^2 \left[ \sqrt{2} \operatorname{Re} \left\{ f(00|111; c, t) \right\} \right] c^2 dc , \quad (2.128)
\]

\[
\gamma_z(t) = \sqrt{4\pi} \int_0^\infty \frac{1}{2} mc^2 \operatorname{Im} \left\{ f(00|111; c, t) \right\} c^2 dc . \quad (2.129)
\]
Another transport property of physical interest is the temperature tensor. This symmetric
tensor is defined by

\[ kT(r, t) = m \langle (e^- < c >)(e^- < c >) \rangle . \]  

(2.130)

In the time-dependent hydrodynamic regime, the temperature tensor can be expanded in powers
of the density gradient:

\[ kT(r, t) = kT^{(0)}(t) + kT^{(1)}(t) \cdot \frac{\nabla n}{n} + \ldots , \]  

(2.131)

where the \( T^{(i)} \) are time-dependent tensors of rank \( i + 2 \). If spatially homogeneous conditions
are assumed in evaluating the temperature tensor, then it must have the following form:

\[ T(t) = \begin{pmatrix}
T_{xx} & T_{xy} & T_{xz} \\
T_{yx} & T_{yy} & T_{yz} \\
T_{zx} & T_{zy} & T_{zz}
\end{pmatrix}, \]

where \( T_{xy} = T_{yx} \), \( T_{xz} = T_{zx} \) and \( T_{yz} = T_{zy} \). The components of the temperature tensor are also
time-dependent quantities and given by:

\[ kT_{xx}(t) = m[< c_x^2 > - < c_x > < c_x >] , \]  

(2.132)

\[ kT_{yy}(t) = m[< c_y^2 > - < c_y > < c_y >] , \]  

(2.133)

\[ kT_{zz}(t) = m[< c_z^2 > - < c_z > < c_z >] , \]  

(2.134)

\[ kT_{xy}(t) = m[< c_x c_y > - < c_x > < c_y >] , \]  

(2.135)

\[ kT_{xz}(t) = m[< c_x c_z > - < c_x > < c_z >] , \]  

(2.136)

\[ kT_{yz}(t) = m[< c_y c_z > - < c_y > < c_z >] . \]  

(2.137)

In order to find the explicit form of these components, it is convenient to express \( c_i, c_{ij} \ (i \neq j) \)
and \( c_i^2 \ (i, j = x, y, z) \) in terms of standard spherical harmonics:

\[ c_x = \frac{i}{\sqrt{2}} \sqrt{\frac{4\pi}{3}} c \left[ Y_1^{(1)}(\hat{e}) - Y_1^{(1)}(\hat{e}) \right] \]

\[ c_y = \frac{1}{\sqrt{2}} \sqrt{\frac{4\pi}{3}} c \left[ Y_1^{(1)}(\hat{e}) + Y_1^{(1)}(\hat{e}) \right] \]

\[ c_z = -i \sqrt{\frac{4\pi}{3}} c Y_0^{(1)}(\hat{e}) . \]  

(2.138)

Employing the coupling rule for the spherical harmonics (2.7) together with the properties of
the Clebsch-Gordan coefficients we have

\[ c_x^2 = \frac{1}{2} \sqrt{\frac{4\pi}{3}} c^2 \left[ \sqrt{\frac{4}{3}} Y_0^{(0)}(\hat{e}) + \sqrt{\frac{4}{15}} Y_0^{(2)}(\hat{e}) - \sqrt{\frac{2}{5}} \{ Y_2^{(2)}(\hat{e}) + Y_2^{(-2)}(\hat{e}) \} \right] \]

\[ c_y^2 = \frac{1}{2} \sqrt{\frac{4\pi}{3}} c^2 \left[ \sqrt{\frac{4}{3}} Y_0^{(0)}(\hat{e}) + \sqrt{\frac{4}{15}} Y_0^{(2)}(\hat{e}) + \sqrt{\frac{2}{5}} \{ Y_2^{(2)}(\hat{e}) - Y_2^{(-2)}(\hat{e}) \} \right] \]

\[ c_z^2 = \sqrt{\frac{4\pi}{3}} c^2 \left[ \frac{1}{3} Y_0^{(0)}(\hat{e}) - \sqrt{\frac{4}{15}} Y_0^{(2)}(\hat{e}) \right] . \]  

(2.139)
Using (2.77) to zeroth order in the density gradient, it follows from (2.138), (2.139) and the definitions (2.132)-(2.136)

\[
kT_{xx}(t) = \sqrt{\frac{4\pi}{3}} \int_0^\infty mc^2 \left[ \frac{1}{\sqrt{3}} f(00|000; c, t) + \frac{1}{\sqrt{15}} f(20|000; c, t) \right] c^2 dc + m \left[ \frac{8\pi}{3} \int_0^\infty c \text{Im}\{f(11|000; c, t)\} c^2 dc \right]^2
\]

(2.140)

\[
kT_{yy}(t) = \sqrt{\frac{4\pi}{3}} \int_0^\infty mc^2 \left[ \frac{1}{\sqrt{3}} f(00|000; c, t) + \frac{1}{\sqrt{15}} f(20|000; c, t) \right] c^2 dc - m \left[ \frac{8\pi}{3} \int_0^\infty c \text{Im}\{f(11|000; c, t)\} c^2 dc \right]^2
\]

(2.141)

\[
kT_{zz}(t) = \sqrt{\frac{4\pi}{3}} \int_0^\infty mc^2 \left[ \frac{1}{\sqrt{3}} f(00|000; c, t) - \frac{2}{\sqrt{15}} f(20|000; c, t) \right] c^2 dc - m \left[ \frac{8\pi}{3} \int_0^\infty c \text{Im}\{f(11|000; c, t)\} c^2 dc \right]^2
\]

(2.142)

\[
kT_{xy}(t) = -\sqrt{\frac{2}{5}} \sqrt{\frac{4\pi}{3}} \int_0^\infty mc^2 \text{Im}\{f(22|000; c, t)\} c^2 dc + \frac{8\pi}{3} m \int_0^\infty c \text{Im}\{f(11|000; c, t)\} c^2 dc \int_0^\infty c \text{Re}\{f(11|000; c, t)\} c^2 dc,
\]

(2.143)

\[
kT_{xz}(t) = \sqrt{\frac{2}{5}} \sqrt{\frac{4\pi}{3}} \int_0^\infty mc^2 \text{Re}\{f(21|000; c, t)\} c^2 dc + \sqrt{\frac{2}{15}} m \int_0^\infty c \text{Im}\{f(11|000; c, t)\} c^2 dc \int_0^\infty c \text{Re}\{f(10|000; c, t)\} c^2 dc,
\]

(2.144)

\[
kT_{yz}(t) = \sqrt{\frac{2}{5}} \sqrt{\frac{4\pi}{3}} \int_0^\infty mc^2 \text{Im}\{f(21|000; c, t)\} c^2 dc - \sqrt{\frac{2}{15}} m \int_0^\infty c \text{Re}\{f(11|000; c, t)\} c^2 dc \int_0^\infty c \text{Im}\{f(10|000; c, t)\} c^2 dc.
\]

(2.145)

In what follows we focus on the distribution function. Our goal is to express the distribution function in a form more amenable for numerical computation and comparison with earlier numerical work. As a first step, we define

\[
F(lm|s\lambda\mu; c, t) = i^{l+\lambda} \left[ \frac{2^{|m|}(2l+1)(l-|m|)!}{4\pi(l+|m|)!} \right]^{1/2} f(lm|s\lambda\mu; c, t).
\]

(2.146)

Using the definition of spherical harmonics (2.1), the distribution function may be written in terms of these moments as follows

\[
f(r, c, t) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \sum_{s=0}^{\infty} \sum_{\lambda=0}^{\infty} \sum_{\mu=-\lambda}^{\lambda} \frac{(-i)^l (-i)^{|m|} (-i)^{m+|m|}/2}{2^{|m|/2}} F(lm|s\lambda\mu; c, t) P_l^{im}\left(\cos \theta\right)e^{i\mu\phi} G_{\mu}^{(s\lambda)} n(r, t).
\]

(2.147)
In this work we are primarily concerned with the spatially homogeneous distribution function

\[ f^{(0)}(c, t) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} f(lm|000; c, t) Y_{m}^{l}. \]  

(2.148)

Using (2.1), (2.146) and (2.147) yields

\[ f^{(0)}(c, t) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} (-i)^{m} F(lm|000; c, t) P_{l}^{m}(\cos \theta)e^{im\phi} \]

\[ = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \tilde{F}(lm|000; c, t) P_{l}^{m}(\cos \theta)e^{im\phi}, \]  

(2.149)

where

\[ \tilde{F}(lm|000; c, t) = (-i)^{m} F(lm|000; c, t) = i^{l} (-i)^{m} \sqrt{(2l+1)(l-m)!} \frac{(l+m)!}{4\pi(l+m)!} f(lm|000; c, t). \]  

(2.150)

Therefore, the spatially homogeneous distribution function may be written as

\[ f^{(0)}(c, t) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} (2 - \delta_{m0}) \left[ \text{Re} \left\{ \tilde{F}(lm|000; c, t) \right\} \cos(m\phi) \right. \]

\[ \left. - \text{Im} \left\{ \tilde{F}(lm|000; c, t) \right\} \sin(m\phi) \right] P_{l}^{m}(\cos \theta). \]  

(2.151)

### 2.6 Steady-state non-hydrodynamic regime

In the steady-state limit with no assumptions on the space-dependence the spherical harmonics decomposition of the Boltzmann equation (2.62) for the configuration of fields in figure (2.1) reduces to the following coupled integro-differential equations:

\[ \sum_{l'=0}^{\infty} \sum_{m'=-l'}^{l'} \left\{ J^{l} \delta_{mm'} \delta_{ll'} - ia(l'm10|lm) < l||\partial_{l}^{[1]}||l' > \delta_{mm'} \right. \]

\[ + \Omega \left\{ \frac{1}{2} \sin \psi \left[ (l-m)(l+m+1)\delta_{mm'+1} - (l+m)(l-m+1)\delta_{mm'-1} \right] - im \cos \psi \delta_{mm'} \right\} \]

\[ - i(l'm10|lm) < l||e^{[1]}||l' > \delta_{mm'} \partial_{z} f_{m'}^{(l')} (z, c) = 0, \]  

(2.152)

where \( a = qE/m \) and \( \Omega = qB/m \) are charged-particle acceleration and cyclotron frequency, respectively. The reduced matrix elements \( < l||\partial_{l}^{[1]}||l' > \) and \( < l||e^{[1]}||l' > \) are given by equations (2.63) and (2.64).

Equation (2.152) constitutes a system of partial-differential equations for the expansion coefficients \( f_{m'}^{(l')} (z, c) \). Note that the spatial gradient term in the Boltzmann equation is retained intact and hence the above system of partial-differential equations represents a boundary value problem. Similar system of partial-differential equations has been recently obtained for an orthogonal configuration of the electric and magnetic fields (Li et al., 2006). Solving the system (2.152) is not an easy task and detailed discussion is deferred to later chapters.
2.6.1 Transport properties in the non-hydrodynamic regime

Transport properties of electrons under general non-hydrodynamic conditions are given by (2.40)-(2.43). In terms of moments $f_{m}^{(l)}(z, c)$, the mean energy and average velocity components are given by:

$$\varepsilon(z) = \sqrt{4\pi} \frac{1}{n(z)} \int_0^\infty \frac{1}{2} mc^2 f_0^{(0)}(z, c) c^2 dc ,$$  \hspace{1cm} (2.153)

$$v_x(z) = \frac{1}{n(z)} \sqrt{\frac{8\pi}{3}} \int_0^\infty \text{Im} \{ f_1^{(1)}(z, c) \} c^2 dc ,$$  \hspace{1cm} (2.154)

$$v_y(z) = \frac{1}{n(z)} \sqrt{\frac{8\pi}{3}} \int_0^\infty \text{Re} \{ f_1^{(1)}(z, c) \} c^2 dc ,$$  \hspace{1cm} (2.155)

$$v_z(z) = -\frac{1}{n(z)} \sqrt{\frac{4\pi}{3}} \int_0^\infty \text{Im} \{ f_0^{(1)}(z, c) \} c^2 dc ,$$  \hspace{1cm} (2.156)

where $n(z)$ is the charged-particle number density given by

$$n(z) = \sqrt{4\pi} \int_0^\infty f_0^{(0)}(z, c) c^2 dc .$$  \hspace{1cm} (2.157)

Note that if electric and magnetic fields are crossed at arbitrary angle, then the average velocity has three independent components.
Chapter 3

The kinetic equations in a Sonine polynomial basis

3.1 Introduction

In previous chapter the hierarchy of kinetic equations for both the time-dependent hydrodynamic (2.93) and steady-state non-hydrodynamic regimes (2.152) was derived by representing the angular component of the velocity dependence of the phase-space distribution function in terms of an expansion in spherical harmonics. Further decomposition of the coefficients $f(lm|sλμ;c,t)$ and $f^l_m(z,c)$ in speed space is our next task. Many options are available for the decomposition of these moments including finite differencing schemes, polynomial expansions, pseudo-spectral methods etc. In traditional kinetic theory, however, the treatment of a speed dependence has been made through the expansion in terms of Sonine polynomials about a variety of Maxwellian-based weighting functions. The combination of spherical harmonics and Sonine polynomials makes the well-known Burnett functions. The Burnett functions have been extensively used in the kinetic theory for both the hydrodynamic and non-hydrodynamic studies (Burnett (1935a; 1935b); Chapman and Cowling (1939); Kumar (1966a; 1966b; 1967); Lin et al. (1979a); Mason and McDaniel (1988); Viehland and Mason (1975; 1978); Ness and Robson (1986; 1988; 1989); Ness (1993; 1994); White (1996); White et al. (1999a; 2002); Li et al. (2002; 2006). Two reasons lie behind their extensive use: first, these functions are eigenfunctions of the linearized Boltzmann collision operator for Maxwellian molecules, and second, they are orthogonal with respect to a Maxwellian weight function in the velocity space.

In case of the electron swarms, two-temperature method (i.e. the weighting function is a Maxwellian at a temperature $T_b$ and not equal to the neutral gas temperature $T_0$ which is a flexible parameter used to optimize convergence) is generally sufficient (Lin et al., 1979a). This method has been further optimized and improved for the time-dependent fields by considering a varying Maxwellian weighting function in time (White (1996)). Such extension of the traditionally two-temperature moment method is required to deal with any temporal variation of the phase space distribution function.
3.2 Time-dependent hydrodynamic regime

3.2.1 Representation of the speed dependence in terms of Sonine polynomials

The speed distribution function is expanded about a Maxwellian at an arbitrary time-dependent temperature $T_b(t)$, in terms of Sonine polynomials. In summary, the expansion of the speed-dependence of the coefficients $f(lm|s\lambda\mu; c, t)$ in (2.93) is given by:

$$f(lm|s\lambda\mu; c, t) = w(\alpha(t), c) \sum_{\nu'=0}^{\infty} F(\nu'lm|s\lambda; \alpha(t), t) R_{\nu'l}(\alpha(t)c) ,$$

where

$$R_{\nu'l}(\alpha(t)c) = N_{\nu'l} \left( \frac{\alpha(t)c}{\sqrt{2}} \right) S_{l+1/2}^{(\nu)} \left( \frac{\alpha^2(t)c^2}{2} \right)$$

$$w(\alpha(t), c) = \left( \frac{\alpha^2(t)}{2\pi} \right)^{3/2} \exp \left\{ -\frac{\alpha^2(t)c^2}{2} \right\}$$

$$\alpha^2(t) = \frac{\frac{m}{kT_b(t)}}{\Gamma(\nu + l + 3/2)}$$

The Sonine polynomials are given by the relation (Kumar, 1966a)

$$S_{l+1/2}^{(\nu)} \left( \frac{\alpha^2(t)c^2}{2} \right) = \sum_{p=0}^{\nu} \frac{1}{p!(\nu - p)!} \frac{\Gamma(\nu + l + 3/2)}{\Gamma(p + l + 3/2)} \left( -\frac{\alpha^2(t)c^2}{2} \right)^p .$$

From the orthogonality of Sonine polynomials, the orthonormality of these R polynomials follows:

$$\int_0^\infty w(\alpha(t), c) R_{\nu'l}(\alpha(t)c) R_{\nu''l}(\alpha(t)c)c^2 dc = \delta_{\nu\nu'} .$$

Substitution of (3.1) into (2.77) yields the full representation of the phase-space distribution function:

$$f(r, c, t) = \sum_{s=0}^{\infty} \sum_{\lambda=0}^{s} \sum_{\mu=-\lambda}^{\lambda} \sum_{\nu=0}^{\infty} \sum_{l=0}^{\infty} \sum_{m=-l}^{l} F(\nu lm|s\lambda\mu; \alpha(t), t) R_{\nu'l}(\alpha(t)c)Y_{m}^{[\nu]}(\hat{c})$$

$$G_{\mu}^{(s\lambda)} n(r, t)$$

$$= w(\alpha(t), c) \sum_{s=0}^{\infty} \sum_{\lambda=0}^{s} \sum_{\mu=-\lambda}^{\lambda} \sum_{\nu=0}^{\infty} \sum_{l=0}^{\infty} \sum_{m=-l}^{l} F(\nu lm|s\lambda\mu; \alpha(t), t) \phi_{m}^{[\nu]}(\alpha(t)c)C_{\mu}^{(s\lambda)} n(r, t) ,$$

where

$$\phi_{m}^{[\nu]}(\alpha(t)c) = R_{\nu'l}(\alpha(t)c)Y_{m}^{[\nu]}(\hat{c})$$

are Burnett functions.
In a normalized Sonine polynomial basis, the symmetry properties of the moments \( f(lm|s\lambda\mu; c, t) \) given by (2.70)-(2.76) and by (2.95) can be written now as follows:

\[
F(\nu lm|s\lambda\mu; \alpha(t), t) = 0 \quad \text{if } |m| < \min\{\lambda, l\},
\]

\[
F(\nu lm|s\lambda\mu; \alpha(t), t) = 0 \quad \text{if } |\mu| > \lambda \text{ or } \lambda > s,
\]

\[
F^*(\nu lm|s\lambda\mu; \alpha(t), t) = (-1)^{l+\lambda+m+\mu}F(\nu l - m|s\lambda - \mu; \alpha(t), t),
\]

\[
F(\nu lm|s\lambda\mu; \alpha(t), t; -\mathbf{E}, \mathbf{B}) = (-1)^{l+\lambda}F(\nu lm|s\lambda\mu; \alpha(t), t; \mathbf{E}, \mathbf{B}),
\]

\[
F(\nu lm|s\lambda\mu; \alpha(t), t; \mathbf{E}, -B_y, B_z) = (-1)^{m+\mu}F(\nu lm|s\lambda\mu; \alpha(t), t; \mathbf{E}, \mathbf{B}),
\]

\[
F(\nu lm|s\lambda\mu; \alpha(t), t; \mathbf{E}, -B, B_y, -B_z) = (-1)^{m+\mu}F(\nu l - m|s\lambda - \mu; \alpha(t), t; \mathbf{E}, \mathbf{B}),
\]

\[
F(000|s\lambda\mu; \alpha(t), t) = \delta_{s0}\delta_{\lambda0}\delta_{\mu0}.
\]

### 3.2.2 Hierarchy of kinetic equations in a Sonine polynomial basis

Substitution of the expansion (3.1) into (2.93), pre-multiplying by \( c^2 R_{\nu l}(\alpha(t)c) \) and integrating over all speeds, converts the hierarchy of kinetic equations (2.93) into a hierarchy of differential matrix equations for the moments \( F(\nu lm|s\lambda\mu; c, t) \)

\[
\sum_{\nu' = 0}^{\infty} \sum_{l' = 0}^{\infty} \sum_{m' = -l'}^{0} \left\{ \delta_{\nu\nu'}\delta_{ll'}\delta_{mm'} + \omega(000; t)\delta_{\nu\nu'}\delta_{ll'}\delta_{mm'} + n_0 J_{\nu\nu'}^{l'} \delta_{ll'}\delta_{mm'} \right\}
\]

\[
+ ia(t)(l' m 0|l m)\alpha(t) < \nu l||K^{[1]}||\nu l' > \delta_{mm'}
\]

\[
+ \frac{q}{m} B(t) \left\{ \sin \psi \left[ \sqrt{(l - m)(l + m + 1)}\delta_{m'm+1} - \sqrt{(l + m)(l - m + 1)}\delta_{m'm-1} \right] \right. 
\]

\[
- i m \cos \psi \delta_{mm'} \left. \right\} F(\nu l'|m'|s\lambda\mu; \alpha(t), t) = X(\nu lm|s\lambda\nu; \alpha(t), t),
\]

where

\[
X(\nu lm|s\lambda\nu; \alpha(t), t) = \sum_{\nu' = 0}^{\infty} \sum_{l' = 0}^{\infty} \sum_{m' = -l'}^{0} \left( \sum_{s = 0}^{\infty} \sum_{s_1 = 0}^{s} \sum_{l_1 = 0}^{l} \sum_{s_1 = 0}^{l} \sum_{l_1 = 0}^{l} \sum_{\lambda_1 = 0}^{\lambda_1} \sum_{\lambda_2 = 0}^{\lambda_2} (\lambda_1 \mu_1 \lambda_2 \mu_2 | \lambda \mu) 
\]

\[
(1 - \delta_{ss_1} \delta_{\lambda_0 \lambda_2})\omega(s - s_1 \lambda_2 \mu_2; t) F(\nu l'|m'|s_1 \lambda_1 \mu_1; \alpha(t), t) \delta_{\nu\nu'}\delta_{ll'}\delta_{mm'}
\]

\[
+ \frac{1}{(\alpha(t))}\sum_{\mu = -s}^{s} \sum_{\lambda_1 = 0}^{\lambda_1} \sum_{\lambda_2 = 0}^{\lambda_2} (l' m'|1 \mu |l m)(l \mu \lambda_1 \mu_1 | \lambda \mu) < \nu l|| \alpha(t)c^{[1]}||\nu l' > F(\nu l'|m'|s - 1 \lambda_1 \mu_1; \alpha(t), t).
\]

The reduced matrix elements appearing in (3.19) and (3.20) are defined as

\[
< \nu l||\alpha(t)c^{[1]}||\nu l' > = \frac{1}{\alpha(t)} \int_{0}^{\infty} R_{\nu l}(\alpha(t)c) < l||c^{[1]}||l' > w(\alpha(t), c) R_{\nu l'}(\alpha(t)c)c^2 dc
\]

and

\[
< \nu l||K^{[1]}||\nu l' > = -\frac{1}{\alpha(t)} \int_{0}^{\infty} R_{\nu l}(\alpha(t)c)\left\{ < l||\partial c||l' > w(\alpha(t), c) R_{\nu l'}(\alpha(t)c) \right\} c^2 dc.
\]
while

\[ J_{\nu \nu'}(\alpha(t)) = \frac{1}{n_0} \int_0^\infty R_{\nu \nu'}(\alpha(t)c)J^l[w(\alpha(t),c)R_{\nu' l}(\alpha(t)c)]c^2 dc \]  

(3.23)
is the collision matrix. The explicit form of the reduced matrix elements (3.21) and (3.22) is given by (Kumar (1967)):

\[
< \nu l || \alpha(t)c^{[1]} || \nu' l' > = \sqrt{\frac{2}{2l+1}} \left[ \frac{\sqrt{l(l+1/2)\delta_{\nu\nu'}d_{l+1} - \sqrt{l(l+1)\delta_{\nu\nu'+1}d_{l'-1}}}}{} - \sqrt{l(l+1)\delta_{\nu\nu'-1}d_{l'-1} + \sqrt{(l+1)(l+3/2)\delta_{\nu\nu'}d_{l'-1}}} \right] 
\]

(3.24)

\[
< \nu l || K^{[1]} || \nu' l' > = \sqrt{\frac{2}{2l+1}} \left[ \sqrt{l(l+1/2)\delta_{\nu\nu'}d_{l+1} - \sqrt{l(l+1)\delta_{\nu\nu'+1}d_{l'-1}}} \right] .
\]

(3.25)

Using the relation

\[
ed^l = \left( \frac{\sqrt{7}}{\alpha(t)} \right)^l \frac{R_{00}(\alpha(t)c)}{N_{0l}},
\]

(3.26)

and the orthonormality condition (3.7), it follows from (2.80) that the expansion coefficients of the spherical form of the continuity equation are given by

\[
\omega(s \lambda \mu ; t) = \frac{1}{\alpha(t)} \sum_{\mu = -1}^1 \sum_{\lambda_1 = 0}^{s-1} (-1)^{\mu} (1\bar{\mu} \lambda_1 \mu - \bar{\mu} \lambda \mu) F(01 - \bar{\mu}|s - 1 \lambda_1 \mu - \bar{\mu}; \alpha(t), t)
\]

\[
- n_0 \sum_{\nu' = 0}^{\infty} J_{00\nu'}^0(\alpha(t))F(\nu'00|s \lambda \mu; \alpha(t), t) .
\]

(3.27)

Alternatively, this expression could be obtained by setting \( \nu = l = m = 0 \) in (3.19) and using (3.24) and (3.25) to evaluate the required reduced matrix elements.

From (3.27), it is obvious that in the presence of non-conservative collisions the \( s_1 = \lambda_1 = \mu_1 = 0 \) term of (3.20) involves a summation over the first row of the collision matrix and the unknown moments \( F(\nu00|s \lambda \mu; \alpha(t), t) \). Therefore, each member of (3.19), (3.20) and (3.27) may be viewed as a system of coupled equations which must be solved in a self-consistent manner. The procedure adopted for solution of this system involves the extraction of the \( s_1 = \lambda_1 = \mu_1 = 0 \) term from the first term of (3.20) containing \( \omega(s \lambda \mu ; t) \) and substitution of (3.27) into (3.20), whereby the reactive collision matrix elements involved can be incorporated into the matrix of coefficients of (3.19). Performing this procedure results in the following hierarchy of doubly infinite coupled partial differential equations for the moments \( F(\nu\nu m|s \lambda \mu; \alpha(t), t) \):

\[
\sum_{\nu' = 0}^{\infty} \sum_{l' = 0}^{\infty} \sum_{m' = -l'}^{l'} \left\{ \partial_t \delta_{\nu \nu'} \delta_{l l'} \delta_{m m'} + \omega(000; t)\delta_{\nu \nu'} \delta_{l l'} \delta_{m m'} + n_0 J_{\nu \nu'}^l \delta_{l l'} \delta_{m m'} 
\right.
\]

\[
+ ia(t)(l' m 10|l m) \alpha(t) < \nu l || K^{[1]} || \nu' l' > \delta_{m m'} + 
\]
where

\[
\begin{aligned}
\hat{X}(\nu \ell \mu |s \lambda \mu; \alpha(t), t) &= \sum_{\nu'=0}^{\infty} \sum_{\ell'=0}^{\infty} \sum_{m'=-\infty}^{\infty} \left[-\frac{1}{\alpha(t)} \sum_{\lambda_1=0}^{s-1} \sum_{\bar{\mu}=-1}^{1} (\ell' m' \bar{\mu} | \ell m) (\nu' | \alpha(t) | c^{[1]} | \nu' |) F(\nu' \ell' m' | s - 1 \lambda_1 \mu - \bar{\mu}; \alpha(t), t)
\right.

\left. \sum_{s_1=0}^{s} \sum_{\lambda_1=0}^{s} \sum_{\mu_1=-s_1}^{s_1} \sum_{\mu_2=-\lambda_2}^{\lambda_2} \omega(s - s_1 \lambda_2 \mu_2 | t) (1 - \delta_{s_1,0} \delta_{\lambda_1,0} \delta_{\mu_1,0}) \right]
\end{aligned}
\]

The rhs no longer contains any unknown information and direct solution of the system can be found. However, the spatially homogeneous member contains unknown information in the coefficient matrix on the lhs, \(\omega(00; t)\), and a self-consistent solution is required. It must be emphasized that in the absence of non-conservative collisions, no such coupling exists and all hierarchy members can be solved for the moments directly (White et al. (2002)).

### 3.2.3 Transport coefficients, properties and distribution function

Using the relation (3.27), the orthonormality of the basis functions (3.7) and definition of the collision matrix (3.23), the explicit form of the bulk transport coefficients in a Sonine polynomial basis are from (2.99)-(2.108):

\[
\alpha(t) = n_0 \sum_{\nu'=0}^{\infty} J_{0,\nu'}^0(\alpha(t)) F(\nu'00|000; \alpha(t), t),
\]

\[
W_x(t) = \frac{\sqrt{2}}{\alpha(t)} \text{Im} \left\{ F(011|000; \alpha(t), t) \right\} - \sqrt{2} \sum_{\nu'=0}^{\infty} n_0 J_{0,\nu'}^0 \text{Im} \left\{ F(\nu'00|111; \alpha(t), t) \right\},
\]

\[
W_y(t) = \frac{\sqrt{2}}{\alpha(t)} \text{Re} \left\{ F(01 - 1|000; \alpha(t), t) \right\} + \sqrt{2} \sum_{\nu'=0}^{\infty} n_0 J_{0,\nu'}^0 \text{Re} \left\{ F(\nu'00|111; \alpha(t), t) \right\},
\]

\[
W_z(t) = -\frac{1}{\alpha(t)} \text{Im} \left\{ F(010|000; \alpha(t), t) \right\} + \sum_{\nu'=0}^{\infty} n_0 J_{0,\nu'}^0 \text{Im} \left\{ F(\nu'00|110; \alpha(t), t) \right\},
\]

73
The spatially homogeneous mean energy from (2.126) is given by

\[ D_{xx}(t) = -\frac{1}{\alpha(t)} \left[ \text{Re} \left\{ F(011|111; \alpha(t), t) \right\} - \text{Re} \left\{ F(01 - 1|111; \alpha(t), t) \right\} \right] + \sum_{\nu' = 0}^{\infty} n_0 J_{0\nu'}^0 \left[ \frac{1}{\sqrt{3}} F(\nu'00|220; \alpha, t) + \frac{1}{\sqrt{6}} F(\nu'00|220; \alpha, t) - \text{Re} \left\{ F(\nu'00|222; \alpha(t), t) \right\} \right], \quad (3.34) \]

\[ D_{yy}(t) = -\frac{1}{\alpha(t)} \left[ \text{Re} \left\{ F(011|111; \alpha(t), t) \right\} + \text{Re} \left\{ F(01 - 1|111; \alpha(t), t) \right\} \right] + \sum_{\nu' = 0}^{\infty} n_0 J_{0\nu'}^0 \left[ \frac{1}{\sqrt{3}} F(\nu'00|200; \alpha, t) + \frac{1}{\sqrt{6}} F(\nu'00|220; \alpha, t) + \text{Re} \left\{ F(\nu'00|222; \alpha(t), t) \right\} \right], \quad (3.35) \]

\[ D_{zz}(t) = -\frac{1}{\alpha(t)} F(010|110; \alpha(t), t) - \sum_{\nu' = 0}^{\infty} n_0 J_{0\nu'}^0 \left[ \frac{1}{\sqrt{3}} F(\nu'00|200; \alpha, t) - \sqrt{\frac{2}{3}} F(\nu'00|220; \alpha, t) \right], \quad (3.36) \]

\[ D_1(t) = \frac{2}{\alpha(t)} \text{Im} \left\{ F(01 - 1|111; \alpha(t), t) \right\} + \sum_{\nu'} n_0 J_{0\nu'}^0(\alpha(t)) 2\text{Im} \left\{ F(\nu'00|220; \alpha(t), t) \right\}, \quad (3.37) \]

\[ D_2(t) = \frac{\sqrt{2}}{\alpha(t)} \left[ \text{Re} \left\{ F(010|111; \alpha(t), t) \right\} - \text{Re} \left\{ F(01 - 1|110; \alpha(t), t) \right\} \right] \]

\[ - \sum_{\nu' = 0}^{\infty} n_0 J_{0\nu'}^0(\alpha(t)) 2\text{Re} \left\{ F(\nu'00|221; \alpha(t), t) \right\}, \quad (3.38) \]

\[ D_3(t) = \frac{\sqrt{2}}{\alpha(t)} \left[ \text{Im} \left\{ F(010|111; \alpha(t), t) \right\} - \text{Im} \left\{ F(01 - 1|110; \alpha(t), t) \right\} \right] \]

\[ - \sum_{\nu' = 0}^{\infty} n_0 J_{0\nu'}^0(\alpha(t)) 2\text{Im} \left\{ F(\nu'00|221; \alpha(t), t) \right\}. \quad (3.39) \]

The explicit form of the off-diagonal elements of the diffusion tensor in a Sonine polynomial basis are from (2.118)-(2.123):

\[ D_{xy}(t) = \frac{1}{\alpha(t)} \left[ \text{Im} \left\{ F(01 - 1|111; \alpha(t), t) \right\} - \text{Im} \left\{ F(011|111; \alpha(t), t) \right\} \right], \quad (3.40) \]

\[ D_{xz}(t) = \frac{\sqrt{2}}{\alpha(t)} \text{Re} \left\{ F(011|110; \alpha(t), t) \right\}, \quad (3.41) \]

\[ D_{yz}(t) = \frac{1}{\alpha(t)} \left[ \text{Im} \left\{ F(01 - 1|111; \alpha(t), t) \right\} + \text{Im} \left\{ F(011|111; \alpha(t), t) \right\} \right], \quad (3.42) \]

\[ D_{yz}(t) = -\frac{\sqrt{2}}{\alpha(t)} \text{Im} \left\{ F(011|110; \alpha(t), t) \right\}, \quad (3.43) \]

\[ D_{zx}(t) = \frac{\sqrt{2}}{\alpha(t)} \text{Re} \left\{ F(010|111; \alpha(t), t) \right\}, \quad (3.44) \]

\[ D_{zy}(t) = \frac{\sqrt{2}}{\alpha(t)} \text{Im} \left\{ F(010|111; \alpha(t), t) \right\}. \quad (3.45) \]

In a similar fashion, using the relation

\[ c^2 = \sqrt{\frac{3}{4\pi}} \frac{\sqrt{3}}{\alpha^2(t)} \left[ R_{00}(\alpha(t)c) - \sqrt{\frac{2}{3}} R_{10}(\alpha(t)c) \right], \quad (3.46) \]

the spatially homogeneous mean energy from (2.126) is given by

\[ \varepsilon(t) = \frac{3}{2} k T_0(t) \left[ 1 - \sqrt{\frac{2}{3}} F(100|000; \alpha(t), t) \right], \quad (3.47) \]
while the energy gradient vector components from (2.127)-(2.129) are given by

\[
\begin{align*}
\gamma_x(t) &= \frac{3}{2} k T_b(t) \left[ \frac{2}{\sqrt{3}} \Im \left\{ F(100|111; \alpha(t), t) \right\} \right], \\
\gamma_y(t) &= \frac{3}{2} k T_b(t) \left[ -\frac{2}{\sqrt{3}} \Re \left\{ F(100|111; \alpha(t), t) \right\} \right], \\
\gamma_z(t) &= \frac{3}{2} k T_b(t) \left[ -\frac{2}{\sqrt{3}} \Im \left\{ F(100|110; \alpha(t), t) \right\} \right].
\end{align*}
\] (3.48 - 3.50)

To obtain the expressions for the components of the temperature tensor (2.139)-(2.144) in a Sonine polynomial basis, we first express \(c\) and \(c^2\) in terms of the R-polynomials (in addition to expression (3.46)):

\[
\begin{align*}
c &= \sqrt{\frac{3}{4\pi}} \frac{1}{\alpha(t)} R_{01}(\alpha(t)c), \\
c^2 &= \frac{\sqrt{15}}{2} \frac{1}{\sqrt{\pi \alpha^2(t)}} R_{02}(\alpha(t)c).
\end{align*}
\] (3.51 - 3.52)

Using (3.46), (3.51) and (3.52) it follows from (2.139)-(2.144) that the components of the temperature tensor are respectively:

\[
\begin{align*}
T_{xx}(t) &= T_b \left\{ 1 - \sqrt{\frac{2}{3}} F(100|000; \alpha(t), t) + \frac{1}{\sqrt{3}} F(020|000; \alpha(t), t) \\
&\quad - \sqrt{2} \Re \left\{ F(022|000; \alpha(t), t) \right\} - \left[ \sqrt{2} \Im \left\{ F(011|000; \alpha(t), t) \right\} \right]^2 \right\}, \\
T_{yy}(t) &= T_b \left\{ 1 - \sqrt{\frac{2}{3}} F(100|000; \alpha(t), t) + \frac{1}{\sqrt{3}} F(020|000; \alpha(t), t) \\
&\quad + \sqrt{2} \Re \left\{ F(022|000; \alpha(t), t) \right\} - \left[ \sqrt{2} \Im \left\{ F(011|000; \alpha(t), t) \right\} \right]^2 \right\}, \\
T_{zz}(t) &= T_b \left\{ 1 - \sqrt{\frac{2}{3}} F(100|000; \alpha(t), t) - \frac{2}{\sqrt{3}} F(020|000; \alpha(t), t) \\
&\quad - \left[ \Im \left\{ F(010|000; \alpha(t), t) \right\} \right]^2 \right\}, \\
T_{xy}(t) &= T_b \left\{ - \sqrt{2} \Im \left\{ F(022|000; \alpha(t), t) \right\} \\
&\quad + \left[ \sqrt{2} \Im \left\{ F(011|000; \alpha(t), t) \right\} \right] \left[ \sqrt{2} \Re \left\{ F(011|000; \alpha(t), t) \right\} \right] \right\}, \\
T_{xz}(t) &= T_b \left\{ \sqrt{2} \Re \left\{ F(021|000; \alpha(t), t) \right\} \\
&\quad + \sqrt{2} \Im \left\{ F(011|000; \alpha(t), t) \right\} \Im \left\{ F(010|000; \alpha(t), t) \right\} \right\}, \\
T_{yz}(t) &= T_b \left\{ \sqrt{2} \Re \left\{ F(021|000; \alpha(t), t) \right\} \\
&\quad - \sqrt{2} \Im \left\{ F(011|000; \alpha(t), t) \right\} \Im \left\{ F(010|000; \alpha(t), t) \right\} \right\}.
\end{align*}
\] (3.53 - 3.58)

Finally, using (2.151) and (3.1) the explicit form of the spatially homogeneous distribution
function in a Sonine polynomial basis is given by

\[
f^{(0)}(c, t) = \sum_{\nu=0}^{\infty} \sum_{l=0}^{\infty} \sum_{m=0}^{l} (2 - \delta_{m0}) \omega(\alpha(t), t) \left[ \text{Re} \left\{ F(\nu lm|000; c, t) \right\} \cos(m\phi) - \text{Im} \left\{ F(\nu lm|000; c, t) \right\} \sin(m\phi) \right] R_{\nu l}(\alpha(t)c) P_{l}^{m}(\cos \theta).
\]

(3.59)

### 3.2.4 Temporal discretization of the hierarchy of kinetic equations

Following the previous work of White (1996) and White et al. (2002) we employ the implicit finite difference scheme to evaluate the partial time derivatives in (3.3.19). Discretizing in time at the \(n\)th time step, each element of the hierarchy is evaluated at the same basis temperature \(T_{b}^{n}\). If the time step is \(\Delta t\), then the partial derivative at the \(n\)th time step is approximated by:

\[
\frac{\partial}{\partial t} F(\nu lm|s\lambda\mu; \alpha(t), t) \bigg|_{\alpha=\alpha_{n}, t=t_{n}} = \frac{F_{n}(\nu lm|s\lambda\mu; \alpha_{n}) - F_{n-1}(\nu lm|s\lambda\mu; \alpha_{n})}{\Delta t},
\]

(3.60)

The quantity \(F_{n-1}(\nu lm|s\lambda\mu; \alpha_{n})\) is expressed in terms of the known quantities \(F_{n-1}(\nu lm|s\lambda\mu; \alpha_{n-1})\) through the linear equation:

\[
F_{n-1}(\nu lm|s\lambda\mu; \alpha_{n}) = \sum_{\nu'=0}^{\nu} A_{\nu \nu'}^{l}(\mu_{nn-1}) F_{n-1}(\nu lm|s\lambda\mu; \alpha_{n-1}),
\]

(3.61)

where

\[
A_{\nu \nu'}^{l}(\mu_{ij}) = \frac{\bar{N}_{\nu l}^{2}}{N_{\nu l}^{2}} \mu_{ij}^{2} \frac{1}{\nu \Gamma(\nu + l + 3/2)} \left( \frac{1 - \mu_{ij}}{\nu - \nu'} \right)!.
\]

(3.62)

\[
\mu_{ij} = \left( \frac{\alpha_{i}}{\alpha_{j}} \right)^{2}.
\]

(3.63)

\[
\bar{N}_{\nu l}^{2} = \frac{2\pi^{3/2}}{\nu \Gamma(\nu + l + 3/2)} = \frac{1}{(\nu!)^{2}} N_{\nu l}^{2}.
\]

(3.64)

Consistency requires

\[
A_{\nu \nu'}^{l}(1) = \delta_{\nu \nu'}.
\]

(3.65)

The relation (3.61) is a direct result of allowing the zeroth order approximation to the phase-space distribution function (or equivalently the basis set of functions) to vary in time if required. The relation (3.61) follows from the linear relationship between the basis functions (modified Sonine polynomials) at different basis temperatures:

\[
R_{\nu l}(\alpha_{i}c) = \sum_{\nu'=0}^{\nu} A_{\nu \nu'}^{l}(\mu_{ij}) R_{\nu' l}(\alpha_{j}c).
\]

(3.66)

Substitution of (3.60) and (3.61) into (3.28) yields at the \(n\)th time step the following hier-
where $R_{\nu\nu'}$ are reduced matrix elements given by (3.21) and (3.22) respectively. Note that the initial equations for the moments $F_{n}(\nu lm|s\lambda\mu;\alpha_{n})$ in terms of Sonine polynomials:

$$
\sum_{\nu'=-\infty}^{\infty} \sum_{\nu=0}^{\infty} \sum_{l'=0}^{\infty} \sum_{m'=0}^{\infty} \left( \delta_{\nu\nu'} \delta_{l'l'} \delta_{mm'} + \Delta t \left[ \omega_{n}(000) \delta_{\nu\nu'} \delta_{l'l'} \delta_{mm'} + n_{0} J_{\nu\nu'}^{l} \delta_{l'l'} \delta_{mm'} \right] + i a_{n} \alpha_{n} (l'm10|lm) < \nu l || K^{[1]} || \nu' l' > \delta_{mm'} \right.
$$

$$
+ \frac{q}{m} B_{n} \left\{ \sin \frac{\psi}{2} \left[ \sqrt{(l-m)(l+m+1)} \delta_{m'm+1} - \sqrt{(l+m)(l-m+1)} \right] \delta_{mm'} \right.
$$

$$
\left. - \left( \nu l || K^{[1]} || \nu' l' > \delta_{mm'} \right. \right) \}
$$

$$
+ n_{0} J_{0\nu'}^{0}(\alpha_{n}) F(\nu lm|000;\alpha_{n})(1 - \delta_{s00} \delta_{\lambda0} \delta_{\mu0}) \delta_{\nu0} \delta_{m0} \right] \left\{ F(\nu' l'm'|s\lambda\mu;\alpha_{n}) = X(\nu lm|s\lambda\nu;\alpha_{n}) , \right. \}
$$

(3.67)

where

$$
X_{n}(\nu lm|s\lambda\mu;\alpha_{n}) = \sum_{\nu'=0}^{\nu} A_{\nu'\nu}(\mu_{mn-1}) F_{n-1}(\nu lm|s\lambda\mu;\alpha_{n-1}) + \Delta t \tilde{X}_{n}(\nu lm|s\lambda\mu;\alpha_{n}) . \right. \}
$$

(3.68)

### 3.3 Steady-state non-hydrodynamic regime

The speed dependence of the expansion coefficients $f_{m}^{(i)}$ appearing in (2.152) are further expanded in terms of Sonine polynomials:

$$
f_{m}^{(i)}(z,c) = \omega(\alpha,c) \sum_{\nu=0}^{\infty} F(\nu lm|\alpha,z) R_{\alpha}(\alpha c) , \right. \}
$$

(3.69)

where $R_{\alpha}(\alpha c)$ is given by (3.2). Substituting Eq. (3.69) into (2.152) and multiplying by $R_{\alpha}(\alpha c)^{2}$, integrating over all speeds, and using the orthogonality of the $F_{\nu l'}(\nu lm|s\lambda\nu;\alpha_{n})$ functions with respect to the Maxwellian weight function (3.7) yields the following system of coupled differential equations for the moments $F(\nu l'm'|\alpha,z)$

$$
\sum_{\nu'=0}^{\infty} \sum_{l'=0}^{\infty} \sum_{m'=0}^{\infty} \left\{ n_{0} J_{\nu' l'}(\alpha) \delta_{l'l'} \delta_{mm'} + \frac{1}{\alpha}(l'm10|lm) \left< \nu l || \alpha c^{[1]} || \nu' l' > \delta_{mm'} \right. \right.
$$

$$
+ \Omega \left\{ \sin \frac{\Psi}{2} \left[ \sqrt{(l-m)(l+m+1)} \delta_{m'm+1} - \sqrt{(l+m)(l-m+1)} \right] \delta_{mm'} \right.
$$

$$
\left. - \left( \nu l || \alpha c^{[1]} || \nu' l' > \delta_{mm'} \right. \right) \}
$$

$$
- i \frac{1}{\alpha} \left( l'm10|lm \right) \left< \nu l || \alpha c^{[1]} || \nu' l' > \delta_{mm'} \partial_{\alpha} \right) \right) \right. \}
$$

(3.70)

where $J^{l}_{\nu m l'}(\alpha)$ is the collision matrix given by (3.24) while $< \nu l || \alpha c^{[1]} || \nu' l' >$ and $< \nu l || K^{[1]} || \nu' l' >$ are reduced matrix elements given by (3.21) and (3.22) respectively. Note that $T_{b}$ is assumed constant in space.
3.3.1 Transport properties in the non-hydrodynamic regime

In terms of the moments $F(\nu lm | \alpha, z)$, the number density, mean energy and average velocity components are respectively:

\[ n(z) = F(000; \alpha, z), \quad (3.71) \]
\[ \varepsilon(z) = \frac{3}{2} kT_b \left[ 1 - \sqrt{\frac{2}{3}} F(100; \alpha, z) \right], \quad (3.72) \]
\[ v_x(z) = \sqrt{\frac{2}{3}} \frac{\text{Im} \left\{ F(011; \alpha, z) \right\}}{F(000; \alpha, z)}, \quad (3.73) \]
\[ v_y(z) = \sqrt{\frac{2}{3}} \frac{\text{Re} \left\{ F(011; \alpha, z) \right\}}{F(000; \alpha, z)}, \quad (3.74) \]
\[ v_z(z) = -\frac{1}{\alpha} \frac{\text{Im} \left\{ F(010; \alpha, z) \right\}}{F(000; \alpha, z)}. \quad (3.75) \]

3.4 Treatment of the collision operator

In this section we consider the determination of the matrix elements of the collision operator $(J_{\nu \nu'})$ from the interaction potential (for ions) and partial cross-sections (for electrons). The derivation of the collision terms is the most complicated aspect in the expansion procedure and requires lengthy mathematical treatments. However, this problem has been addressed in comprehensive fashion over the last 40 years and hence the theory and associated numerical procedures are well documented in the standard literature (Kumar (1966a; 1966b; 1967), Lin et al. (1979a), Ness and Robson (1985; 1986)). It is not the aim of this thesis to detail such investigations, but rather to outline the collision operators employed and highlight some important features in relation to collision matrices.

In this section a representation of the conservative collision operator is given in a Burnett function basis. Substitution of (3.9) into the rhs of the Boltzmann equation, pre-multiplying by $R_{\nu l} (\alpha(t)c) Y_{m}(\hat{c})$ and integrating over all velocities yields

\[ \int \Phi_{m}^{[\nu \mu]}(\alpha(t)c) J(f) \Phi_{m'}^{[\nu' \mu']}(\alpha(t)c) dc \]
\[ = n_0 \sum_{s=0}^{\infty} \sum_{\lambda=0}^{\infty} \sum_{\mu=0}^{\infty} \sum_{\nu=0}^{\infty} \sum_{\nu'=0}^{\infty} \sum_{m'=0}^{m} <\nu lm | J | \nu' l' m'> F(\nu' l' m' | s \lambda \mu; \alpha(t), t) C^{(s \lambda \mu)}(\nu; \alpha(t), t) n(r, t), \quad (3.77) \]

where

\[ <\nu lm | J | \nu' l' m'> = \frac{1}{n_0} \int \Phi_{m}^{[\nu \mu]}(\alpha(t)c) J \left[ \omega(\alpha(t), c) \Phi_{m'}^{[\nu' \mu']}(\alpha(t)c) \right] dc, \quad (3.78) \]

defines the collision matrix in a Burnett function basis. As we mentioned previously in Section (2.1), the charged particle-neutral molecule interactions are assumed to proceed via central forces while the distribution of neutral molecule velocities is spatially uniform, stationary and isotropic.
in velocity space. Hence the collision matrix is diagonal in \(l\) and \(m\) indices and independent of the latter
\[
<\nu l m|J|\nu' l' m'> = J_{\nu l}(\alpha(t))\delta_{\nu\nu'}\delta_{mm'} .
\] (3.79)

Therefore, the determination of the collision matrix reduces to representing the reduced matrix element \(J_l\) in a normalized Sonine polynomial basis:
\[
J_l(\alpha(t)) = \frac{1}{n_0} \int_0^\infty R_{\nu l}(\alpha(t)c)J_l[\omega(\alpha(t),c)R_{\nu l}(\alpha(t)c)]c^2 dc .
\] (3.80)

The collision matrix can be separated into conservative and non-conservative parts, respectively
\[
J_l(\alpha(t)) = C J_l(\alpha(t)) + R J_l(\alpha(t)) ,
\] (3.81)

where \(C J_l(\alpha(t))\) and \(R J_l(\alpha(t))\) represent the conservative and reactive components of the collision matrix for the interaction of the swarm particles with the \(i\)-th species of neutral molecules.

The charged swarm particles are assumed structureless and spinless, while the neutral molecules in each species can exist in internal states characterized by the quantum number \(j\) corresponding to energy level \(\epsilon_j\) (for simplicity we neglect the degeneracy of internal states). We also neglect any orienting effects exerted by the electric field on polar neutral molecules. The neutral molecule velocities are denoted by \(c_o\), their mass and number density by \(m_o\) and \(n_o\), respectively, and their distribution function by \(f_{oj}(c_o)\). The velocity distribution of neutral species in the \(j\)-th internal state can be characterized by a spatially uniform Maxwellian at time-independent temperature \(T_o\):
\[
f_{oj}(c_o) = n_o \left(\frac{m_o}{2\pi k T_o}\right)^{3/2} \exp\left(-\frac{1}{2}\frac{m_o c_o^2}{k T_o}\right)
\] = \(n_o\omega(\alpha_o, c_o)\),
\] (3.82)

where
\[
\alpha_o = \frac{m_o}{k T_o} .
\] (3.83)

The number density of the neutral molecules in the \(j\)-th internal state is given by
\[
\frac{n_o j}{Z_o} \exp\left(-\frac{\epsilon_j}{k T_o}\right) ,
\] (3.84)

where
\[
Z_o = \sum_j \exp\left(-\frac{\epsilon_j}{k T_o}\right) ,
\] (3.85)

is the partition function.

3.4.1 Conservative collision matrix

Our starting point is a generalized form of the Wang Chang et al. (1964) total collision operator:
\[
C J(f) = \sum_{jk} \int \left[ f(r, c, t)f_{oj}(c_o) - f'(r, c', t)f_{ok}(c_o') \right] \sigma(jk; g\chi)d\hat{g}dc_o .
\] (3.86)
The primes in (3.86) mean postcollision variables and \(\sigma(jk; g\chi)\) is the differential cross section describing the scattering of a swarm particle of velocity \(c\), from a neutral molecule in the \(j\)-th internal state of velocity \(c_o\). After an inelastic collision, the neutral molecule can undergo a transition from state \(j\) to \(k\) and the relative speed \(\left(g = c - c_o\right)\) changes from \(g\) to \(g'\):

\[
\frac{1}{2} \mu g'^2 = \frac{1}{2} \mu g^2 + \epsilon_j - \epsilon_k ,
\]

where

\[
\mu = \frac{mm_o}{m + m_o} ,
\]

is the reduced mass. We note that if \(k = j\) then the interaction is elastic while if \(k > j\) or \(k < j\) then the interactions are inelastic and superelastic respectively. In a superelastic collision the relative speed is actually increased following a collision. Geometrically, the differential cross section is dependent solely on the scattering angle \((\chi)\) in the centre of mass frame and hence it is independent of the planes formed by the initial and final relative velocities. Thus the differential cross section can be expanded as:

\[
\sigma(jk; g\chi) = \sum_{\lambda\mu} \sigma_{\lambda}(jk; g) Y^{(\lambda)}_{\mu}(\hat{g}) Y^{(\lambda)}_{\mu}(\hat{g'}) ,
\]

where

\[
\sigma_{\lambda}(jk; g) = 2\pi \int_{-1}^{1} \sigma(jk; g\chi) P_l(\cos \chi)d(\cos \chi)
\]

define the partial cross sections. For isotropic scattering we note that

\[
\sigma_{\lambda}(jk; g) = 0 \quad \text{for} \quad l \geq 1
\]

and all transport is governed by the total cross section

\[
\sigma_o(jk; g) = 2\pi \int_{-1}^{1} \sigma(jk; g\chi)d(\cos \chi)
\]

As explained elsewhere (Kumar (1966a; 1966b; 1967); Lin et al. (1979a); Ness and Robson (1986); Ness (1985); White (1996)), the matrix elements of the conservative collision operator in a Burnett function basis are given by

\[
C^l_{\nu\nu'}(\alpha(t)) = \sum_{l_{\nu\nu'}a} \sum_p <l_{\nu\nu'}l_{\nu\nu'}a; p > \left( \frac{m}{m + m_o} \right)^p C^l_{\nu\nu'}(jk) ,
\]

where

\[
C^l_{\nu\nu'}(jk) = \sum_{jk} \frac{n_{\nu\nu'}}{m_{\nu\nu'}} C^l_{\nu\nu'}(jk) ,
\]

The conservative interaction integrals

\[
C^l_{\nu\nu'}(jk) = \int_0^\infty w(\gamma g) R_{\nu\nu'}(\gamma g) \left[ R_{\nu\nu'}(\gamma g) \sigma_j(jk; g) - R_{\nu\nu'}(\gamma g') \sigma_k(jk; g') \right] g^3dg .
\]

are by now well established in kinetic theory (Kumar (1966a; 1966b; 1967); Lin et al. (1979a); Ness and Robson (1985)). These quantities represent the matrix elements of the partial cross
sections $\sigma_j(k; g)$ with respect to an R polynomial basis. The mass dependence is contained solely in the mass ratio $(m/(m + m_o))$. The explicit expression for the brackets $< l\nu\nu'|l_a\nu_a\nu_b;p >$ and associated ‘selection rules’ for the indices are given by (Lin \textit{et al.} (1979a); Ness (1985); White (1996)) and will not be repeated here. In summary, for electron or light ion swarms considered in this thesis it is sufficient to truncate (3.93) to first order in the mass ratio. Applying the explicit expressions for the brackets $< l\nu\nu'|l_a\nu_a\nu_b;p >$ we have

\begin{equation}
< l\nu\nu'|l_a\nu_a\nu_b;0 > = \delta_{ll_a} \delta_{\nu\nu_a} \delta_{\nu\nu_b} \\
< l\nu\nu'|l_a\nu_a\nu_b;1 > = -(\nu + l + \nu')\delta_{ll_a} \delta_{\nu\nu_a} \delta_{\nu'\nu_b} \\
+ \frac{2l}{2l + 1} \frac{(\nu + l + 1/2)(\nu' + l + 1/2)}{(\nu' + l + 3/2)(\nu + l + 1/2)} \delta_{ll_{a+1}} \delta_{\nu\nu_a} \delta_{\nu'\nu_b} \\
+ \frac{2(l + 1)}{2l + 1} \frac{\sqrt{\nu}\delta_{ll_a} \delta_{\nu\nu_a+1} \delta_{\nu'\nu_b+1}}{\sqrt{\nu'}(\nu' + l + 3/2)\delta_{ll_a} \delta_{\nu\nu_a} \delta_{\nu'\nu_b}} \\
+ \frac{2(l + 1)}{2l + 1} \frac{\sqrt{\nu')(\nu' + l + 3/2)}{\sqrt{\nu}(\nu + l + 1/2)} \delta_{ll_a} \delta_{\nu\nu_a+1} \delta_{\nu'\nu_b+1} \\
- \frac{2l}{2l + 1} \frac{\sqrt{\nu}(\nu + l + 1)}{\sqrt{\nu'}(\nu' + l + 3/2)} \delta_{ll_{a-1}} \delta_{\nu\nu_a+1} \delta_{\nu'\nu_b} \\
\end{equation}

(3.97)

3.4.2 Non-conservative collision matrix

In this section the collision matrices for non-conservative processes are considered. Collisions in which the number of electrons changes either being produced or removed are regarded as non-conservative. Electron impact ionization, attachment, electron induced detachment from negative ions, and electron-ion recombination fall into this category. In this thesis, we investigate the processes of electron attachment and electron impact ionization. These processes affect both the chemical and physical composition of the interacting particles and play a significant role on the formation of distribution function and transport properties.

3.4.2.1 Attachment collision matrix

A generalized form of the attachment collision operator proposed by Ness and Robson (1986) is assumed in this thesis:

\begin{equation}
\tilde{A}_j(f) = \left[ \sum \int f_{oj}(c_o) g\sigma_A(j; g) dc_o \right] f(r, c, t)
\end{equation}

(3.98)

\begin{equation}
\tilde{A}_j(f) = \sum \nu_A(j; c) f(r, c, t)
\end{equation}

(3.99)

where $\sigma_A^j(j; g)$ and $\nu_A^j(j; c)$ are respectively the total attachment cross-section and attachment collision frequency for an electron to a neutral molecule of the $i$th species in the $j$th state. We note that in an attachment collision there is no scattering of the electron and subsequently there is no restituting component of the collision operator in (3.98). To zeroth order in the mass ratio we observe

\begin{equation}
\nu_A^i(j; c) = n_{i0}^j c\sigma_A^j(j; c)
\end{equation}

(3.100)
As shown elsewhere (Ness and Robson (1985; 1986)), the matrix elements of the attachment collision operator are given as follows:

\[ A^I_{J
u
u'}(\alpha(t)) = \sum_{l_a\nu_a\nu_b} \sum_{\nu} <l\nu\nu'|l_a\nu_a\nu_b;p> \left( \frac{m}{m+m_o} \right)^p A^I_{\nu_a\nu_b} \, , \tag{3.101} \]

where

\[ A^I_{\nu_a\nu_b}(i) = \sum_j \frac{n_o j}{n_o} A^I_{\nu_a\nu_b}(j) . \tag{3.102} \]

The attachment interaction integrals for neutral molecules in the \( j \)-th internal state are given by

\[ A^I_{\nu_a\nu_b}(j) = \int_0^\infty w(\gamma g)R_{\nu_a\nu_b}(\gamma g)\sigma_A(j;g)g^3dg \, , \tag{3.103} \]

while the bracket coefficients in (3.101) are given by White (1996).

### 3.4.2.2 Ionization collision matrix

If we excite a molecule (or atom) to the ground state of a singly charged ion, then ionization of the molecule (or atom) is said to have occurred and an additional electron is free to leave the target particle. A typical example of this process can be written as:

\[ e + A \rightarrow e + e + A . \tag{3.104} \]

Obviously, the dynamics of an ionization collision is considerably more complicated than that of attachment. After an ionization collision, we have a three body problem, in that the available energy and momentum is to be divided between the molecule (or atom) and two electrons. This is not an easy task, but if one assumes the mass of molecule (or atom) to be infinitely heavy then the motion of the molecule throughout the duration of the collision can be neglected. Consequently, the available energy and momentum after ionization can be partitioned between the scattered and ejected electrons. Taking these restrictions into account and following the previous works of Ness (1985) and Ness and Robson (1986), the following general form of the ionization collision operator follows:

\[ I^J(f) = \sum_j n_o j \left\{ \sigma_I(j;c)f(r,c,t) - 2\int c' \sigma_I(j;c')B(c,c';j)f(r,c',tdc' \right\} , \tag{3.105} \]

where \( \sigma_I(j;c') \) is the total cross section for the \( j \)-th ionization channel while \( B(c,c';j) \) denotes the probability density that divides the available momentum between the ejected and scattered electron for the \( j \)-th channel. In particular \( B(c,c';j)dc \) represents the probability that one of the two electrons post-collision has a velocity with \( dc \) of \( c \), given the incident electron has velocity \( c' \). The probability density must satisfy

\[ \int B(c,c';j)dc = 1 \, , \tag{3.106} \]

and

\[ B(c,c';j) = 0 \quad \text{if} \quad c' - c < \epsilon_I(j) \, , \tag{3.107} \]
where $\epsilon'$ and $\epsilon$ are the incident and post-ionization energy of the electrons and $\epsilon_I(j)$ is the ionization potential of the $j$th channel. The factor of 2 in front of the second term on the rhs of (3.105) arises because after each ionization collision there are two indistinguishable electrons. If there is more than one ionization process, than the rhs of (3.105) will involve a summation over all ionization channels. The quantity $2B(c,c';j)\sigma_I(\epsilon')$ may be thought of as “differential” ionization cross section (Ness and Robson, 1986). If we assume scattering occurs via central forces then

$$B(c,c';j) = B(c,c';\hat{c} \cdot \hat{c}';j)$$ (3.108)

$$= B(c,c';\cos \chi';j)$$ (3.109)

$$= \sum_{\lambda \mu} B_\lambda(c,c';j)Y_\mu^\lambda(\hat{c})Y_\mu^\lambda(\hat{c}')$$ , (3.110)

where

$$B_l(c,c';j) = 2\pi \int_{-1}^{1} B(c,c';j) P_l(\cos \chi')d(\cos \chi')$$ , (3.111)

and $\chi'$ is the angle between the scattered or ejected electron with velocity $c$ and the incident electron velocity $c'$ for the $i$th neutral species. The ionization collision matrix in the Burnett function basis corresponding to (3.105) can be written in the form:

$$^{I}J(\alpha(t)) = ^{I}\tilde{U}_{\nu \nu'} - ^{I}\tilde{U}_{\nu \nu'} ,$$ (3.112)

where

$$^{I}\tilde{U}_{\nu \nu'} = \sum_j \frac{n_{oj}}{n_o} ^{I}\tilde{V}_{\nu \nu'}(j) ,$$ (3.113)

$$^{I}\tilde{V}_{\nu \nu'} = \sum_j \frac{n_{oj}}{n_o} ^{I}\tilde{V}_{\nu \nu'}(j) ,$$ (3.114)

and

$$^{I}\tilde{V}_{\nu \nu'}(j) = \int_0^\infty w(\alpha(t),c)R_{\nu \mu}(\alpha(t)c)\sigma_I(j;c)R_{\nu' \mu}(\alpha(t)c)c^3 dc ,$$ (3.115)

$$^{I}\tilde{V}_{\nu \nu'}(j) = \int_0^\infty w(\alpha(t),c)R_{\nu \mu}(\alpha(t)c) \left\{ 2\sigma_I(j';c')B_l(c,c';j) \right\} R_{\nu' \mu}(\alpha(t)c')(c')^3 c'^2 dc' dc .$$ (3.116)
Chapter 4

Numerical considerations of the decomposed Boltzmann equation solutions

4.1 Numerical solutions of the hierarchy of moment equations in the time-dependent hydrodynamic regime

In this section we examine the form and solution of the hierarchy (3.67). By doing so, we make a further generalization with respect to the numerical aspects associated with the works of White (1996) and White et al. (1995; 1998; 1999b). In these previous works the Boltzmann equation was numerically solved for the time-dependent electric field only case. We try to complement these previous works by a comprehensive description of numerical aspects for the most general case assuming the active role of both the time-dependent electric and magnetic fields crossed at arbitrary angle and with arbitrary phase difference when non-conservative collisions are present.

Let us consider the structure and form of the hierarchy (3.67). We observe that each member of the hierarchy (3.67) represents a doubly infinite set of coupled complex equations for the moments $F_n(\nu l m|s \lambda \mu; \alpha_n)$. In matrix form each member at the $n$-th time step can be expressed as follows:

$$ ^n\mathbf{M}(s \lambda \mu)^n \mathbf{F}(s \lambda \mu) = ^n \mathbf{X}(s \lambda \mu), $$

where the elements of these matrices and vectors are given by

$$ ^n\mathbf{M}(s \lambda \mu)_{\nu \nu'}^{\nu' \mu \mu'} = \begin{cases} \delta_{\nu \nu'} \delta_{\nu' \nu'} \delta_{\mu \mu'} + \Delta t \left[ \omega_n(000) \delta_{\nu \nu'} \delta_{\nu' \nu'} \delta_{\mu \mu'} + n_0 I_{\nu \nu'}^{\nu' \nu} \delta_{\mu \mu'} ight] \\
+ i a_n \alpha_n (l' m 10|l m) < \nu l || K^{[1]} || \nu' l' > \delta_{\mu \mu'} \\
\end{cases} $$

84
\[+ \frac{q}{m} B_n \left\{ \frac{\sin \psi}{2} \left[ \sqrt{(l - m)(l + m + 1)} \delta_{m'm + 1} - \sqrt{(l + m)(l - m + 1)} \delta_{m'm - 1} \right. \right. \]
\[- \left. \left. - \imath m \cos \psi \delta_{m'm'} \right\} \right\} \delta_{\nu'\nu} \delta_{\nu'0} - n_0 J^0_{\nu'}(\alpha_n) F(\nu l m | 000; \alpha_n)(1 - \delta_{\alpha 0} \delta_{\lambda 0} \delta_{\mu 0}) \delta_{\nu'0} \delta_{m'm'} \}, \tag{4.2} \]

\[\left[ ^n F(s\lambda\mu) \right]^{l,m}_{\nu} = F_n(\nu l m | s\lambda\mu; \alpha_n), \tag{4.3} \]
\[\left[ ^n X(s\lambda\mu) \right] = X_n(\nu l m | s\lambda\mu; \alpha_n). \tag{4.4} \]

Each element of the coefficient matrix \(^n M(s\lambda\mu)\) is defined by the sextuplet \((\nu, \nu', l, l', m, m')\) and \(^n M(s\lambda\mu)\) may be viewed as a matrix of matrices, exhibiting a block structure. These blocks are defined by the quadruplet \((l, l', m, m')\) while individual elements within each block are defined by the pair \((\nu, \nu')\). The quantities \(^n F(s\lambda\mu)\) and \(^n X(s\lambda\mu)\) are defined by the pair \((l, m)\) while the individual elements are defined by the \(\nu\) index and hence these quantities may be viewed as a vector of vectors.

In what follows the block structure of the coefficient matrix is examined. The collision matrix is diagonal in both the \(l\) and \(m\) indices. The electric field terms are both sub-diagonal and super-diagonal in the \(l\) indices and diagonal in the \(m\) index. The matrix elements of the normal component of the magnetic field are diagonal in both the \(l\) and \(m\) indices while the parallel component is diagonal in \(l\) index but sub-diagonal and super-diagonal in the \(m\) index. The time-derivative operator is diagonal in both the \(l\) and \(m\) indices. When considering the structure of each block, one may observe certain structure within \(\nu\) indices. The time-derivative operator is diagonal in the \(\nu\)-index. The elements of the electric field matrix blocks are diagonal in \(\nu\) in the super-diagonal \(l\)-blocks and super-diagonal in \(\nu\) in the sub-diagonal \(l\)-blocks. All magnetic field matrix blocks are diagonal in the \(\nu\) index. Thus the coefficient matrix \(^n M(s\lambda\mu)\) can be represented in the following form:

\[ ^n M = \begin{bmatrix}
I + \Delta t ^n A^0 & -\Delta t ^n \Delta_0^1 & 0 & \ldots & \ldots \\
-\Delta t ^n \Delta_0^2 & I + \Delta t ^n (A^1 + ^n L_{11}) & -\Delta t ^n \Delta_0^2 & 0 & \ldots \\
0 & -\Delta t ^n \Delta_2^1 & I + \Delta t ^n (A^2 + ^n L_{22}) & -\Delta t ^n \Delta_2^1 & 0 & \ldots \\
\vdots & \vdots & \vdots & \vdots & \vdots & \ddots
\end{bmatrix} \tag{4.5} \]

where

\[ [I]^{m m'}_{\nu' \nu} = \delta_{\nu' \nu} \delta_{m m'} \tag{4.6} \]

\[ [^n A^1]^{\nu' \nu} = \left\{ \omega_n(000) \delta_{\nu' \nu} \delta_{\lambda' \lambda} \delta_{m m'} + n_0 J^0_{\nu'} \delta_{\nu' \nu} \delta_{m m'} \right. \]
\[- \left. - n_0 J^0_{\nu'}(\alpha_n) F(\nu l m | 000; \alpha_n)(1 - \delta_{\alpha 0} \delta_{\lambda 0} \delta_{\mu 0}) \delta_{\nu'0} \delta_{m'm'} \right\}, \tag{4.7} \]

\[ [^n \Delta_0^1(m)]_{\nu' \nu} = \imath a_n \alpha_n (l' m 10 | m) < \nu | l K^{[1]} | \nu' l' > \delta_{m m'}, \tag{4.8} \]

\[ [^n L_{11}(m, m')]_{\nu' \nu} = \frac{q}{m} B_n \left\{ \frac{\sin \psi}{2} \left[ \sqrt{(l - m)(l + m + 1)} \delta_{m'm + 1} - \sqrt{(l + m)(l - m + 1)} \delta_{m'm - 1} \right. \right. \]
\[- \left. \left. - \imath m \cos \psi \delta_{m m'} \right\} \right\} \delta_{\nu' \nu} \delta_{\nu'0}. \tag{4.9} \]
Note that the form of the coefficient matrix $M(s\lambda\mu)$ does not depend on the $s$, $\lambda$ and $\mu$ indices. However, the elements of the coefficient matrix are dependent on these indices. To calculate the non-conservative corrections up to and including the bulk diffusion coefficients requires solution of the following members of the hierarchy: $(s\lambda\mu)=(0,0,0), (1,1,0), (1,1,1), (2,0,0), (2,2,0), (2,2,1), (2,2,2)$. In the absence of non-conservative collisions, however, it is sufficient only to solve the members of the hierarchy up to first order in the density gradients, to determine all quantities of interest. As remarked previously, in contrast to steady-state, the spatially homogeneous member of the hierarchy (3.67) in association with the reaction rate $\omega_n(000)$ represent a doubly infinite set of coupled non-linear equations for the moments $F_n(\nu l m|000; \alpha_n)$. This system is solved iteratively using the similar technique initially developed by White (1996) and White et al. (1998; 1999b).

From (4.5) to (4.9) we see that the coefficient matrix $M(s\lambda\mu)$ is a tridiagonal in the $l$-index, with diagonal elements generally full, while sub- and super-diagonal elements are sparse. The unknown moments $F_n(\nu l m|s\lambda\mu; \alpha_n)$ are determined via direct numerical inversion of the coefficient matrix $M(s\lambda\mu)$. If the sparseness of the coefficient matrix is taken into account, the computation time can be significantly reduced. In the present code the sparseness of the coefficient matrix is exploited using a public domain Y12M system of sparse matrix inversion routines (Zlatev et al., 1981).

### 4.1.1 The convergence criterion and choice of basis parameters

Another important aspect associated with the numerical calculation concerns truncation of the velocity space indices $(\nu, l, m)$ and choice of basis temperatures. In this thesis these three indices are truncated independently at $\nu_{\text{max}}$, $l_{\text{max}}$ and $m_{\text{max}}$ (provided $m_{\text{max}} \leq l_{\text{max}}$) until some convergence criterion in the transport coefficients is satisfied. No upper limits is fixed on the $\nu$ or the $l$ indices and hence the present approach may be viewed as a true multi-term solution. Generally speaking, large deviations from spherical symmetry in velocity space lead to large $l_{\text{max}}$, while large $\nu_{\text{max}}$ is indicative of a significant departure of speed distribution from a Maxwellian at basis temperature $T_b$. It should be noted that although the $m$-index is subject to the restriction $-l \leq m \leq l$, for practical purposes we are free to truncate the $m$ index at some value $|m_{\text{max}}| \leq l_{\text{max}}$. In other words, for numerical purposes the $m$ index can be treated as a pseudo-independent index. Our ability to truncate the $m$ summation dramatically reduces the matrix size and hence decreases the computation time. This can be of great help under conditions that favor anisotropy of the velocity distribution function where large number of spherical harmonics must be used. Under steady-state conditions, it was shown by White et al. (1999) that for some field orientations, magnetic field strengths and gas types, the convergence in the $m$ index is rapidly increased although the velocity distribution function exhibits a remarkable anisotropic feature.
Thus numerically, the phase-space distribution function is approximated by:

\[
f(r, c, t) = w(\alpha(t), c) \sum_{s=0}^{2} \sum_{\lambda=0}^{\nu_{\text{max}}} \sum_{\mu=-\lambda}^{\lambda} \sum_{l=0}^{l_{\text{max}}} \sum_{m=-l}^{l} F(\nu l m | s \lambda \mu; \alpha(t), t) R_{\nu l}(\alpha(t), c) Y_{l m}^{(s \lambda)}(\mathbf{c}) G_{\mu}^{(s \lambda)} n(r, t).
\]

(4.10)

The success of the above expansion is dependent on the choice of the weight function. As discussed in previous chapters, good success has been obtained in describing electron kinetics in time-dependent electric fields by using the ‘two-temperature’ theory in which the velocity distribution function is expanded about a spherically symmetric Maxwellian velocity distribution at some arbitrary and time dependent basis temperature \(T_b(t)\). It should be noted that there are many techniques for estimating \(T_b\) within the two-temperature theory (White et al., 2002) but the most efficient method for electrons is to leave it as a entirely flexible parameter, used to optimize convergence. In general, a single \(T_b\) is sufficient only to ensure the convergence over a limited range of \(E/n_0\) or equivalently \(\varepsilon\). Hence in time-dependent situations where the field (or mean energy) falls outside these limits, the use of a single basis temperature will in general fail. In addition, the presence of time-dependent magnetic field at arbitrary angle and phase with respect to the electric field can induce the additional oscillatory-type behavior in some transport coefficients and hence the following conditions when choosing a scheme for computing \(T_b\) at each time step must be satisfied: (i) the scheme for computing \(T_b\) must be fully automated; (ii) the scheme must be self-consistent (pre-determined choices of \(T_b(t)\) are inefficient and in general inadequate); and (iii) the scheme must minimize the number of basis temperatures used since the evaluation of the collision matrix for each \(T_b\) is computationally expensive.

We have adopted here the scheme for computing \(T_b\) initially developed by White (1996). It is relatively easy to implement this scheme within numerical code and in what follows we briefly sketch its important steps. At a given time step, an initial estimate of the basis temperature is assumed to be that from the previous time step. The transport coefficients are then calculated for this basis temperature over a range of \(\nu_{\text{max}}\) values. The convergence in the \(\nu\) index is then checked on these transport coefficients. It is important to note that number of transport coefficients used in the convergence checks must be more than one. As pointed out by White (2001), different transport coefficients have different rates of convergence depending on the cross sections and other conditions. As an illustrative example, it was found that the longitudinal diffusion coefficient has the slowest rate of convergence for a model gas of hard spheres (White, 2001). In addition, in this thesis both types of transport coefficients, bulk and flux, are considered. The differences between these two sets of transport coefficients can be sometimes quite large. This suggests that both types of transport coefficients must be included in the convergence checks. For practical purposes, in the present numerical code the mean energy, bulk and flux drift velocity components and bulk and flux diagonal elements of the diffusion tensor are used in the convergence checks. The convergence tolerance of each transport coefficient is in general set to 0.5%. However, in some cases this accuracy criterion has to be weakened on some transport coefficients. In any case, whenever the accuracy of transport coefficient was called into question, the independent Monte Carlo checks have been carried out in order to check the solution of the Boltzmann equation.
If the convergence criteria are not satisfied, then a new $T_b$ is chosen and the convergence checks are repeated. The basis temperatures are varied in some systematic manner until the above convergence criteria are satisfied. As remarked previously, many options are available for the variation of $T_b$. In the present code, at the $k$th time step, the basis temperature is modified, according to $kT_b = \rho_k^{-1}T_b$, where $\rho_k$ is a self-adjustable parameter. As an illustrative example, in Figure 5.1 we illustrate the variation of $T_b$ of 1000 K. One immediately notices that the amplitude of variation increases with number of $T_b$ iterations. The number of iterations and choice of the proportionality coefficient $\rho_k$ are dependent on the system investigated.

![Figure 4.1: The variation of the basis temperature of 1000 K as a function of number of iterations.](image)

In general a large $\nu_{\text{max}}$ is indicative of a significant departure of speed distribution from a Maxwellian at basis temperature $T_b$. Convergence is dependent on the nature of the interactions and the choice of the basis temperatures. For a given system, the convergence in the $\nu$-index may vary in time according to the time variation in the type of predominant collisional processes. For a majority of gases and time-dependent electric and magnetic fields considered in this thesis, $\nu_{\text{max}}$ is predefined constant within the range of 40-90. In general, this technique allows to specify the accuracy of the transport coefficients in the $\nu$-index for a defined $l_{\text{max}}$.

When considering the convergence in the $l$-index the following strategy is applied. The convergence in the $l$-index is followed over the whole temporal profile of the transport properties/coefficients. It is assumed that $l_{\text{max}}$ corresponds to the maximum value required for dc steady-state systems over the range of fields up to the field amplitude. If the convergence criteria are not satisfied, the value of $l_{\text{max}}$ is then incremented and the whole procedure is repeated. Like the $\nu$-index convergence, for a given system, the convergence in the $l$-index may vary in time according to the time variation in the energy and hence the type of predominant collisional processes.

This ends our general discussion of the hydrodynamic kinetic theory relevant to the calcu-
lation of swarm transport coefficients and properties in time-dependent electric and magnetic fields and the discussion associated with the numerical solution techniques. In later chapters, the numerical code is employed to a series of model and real, conservative and non-conservative gases for applied dc and ac electric and magnetic fields.

4.2 Numerical solution of the moment equations in the steady-state non-hydrodynamic regime

In this chapter we consider the numerical solution of a hierarchy of coupled differential equations (3.70) to obtain all transport properties under non-hydrodynamic conditions. Following the previous works of Li (2002; 2006) the boundary conditions at the source and in the infinity are specified. We discuss in detail a technique for numerical discretization in configuration space, that is on the borderline between pseudo-spectral and finite difference methods. The unknown spatially dependent moments are then determined via direct numerical inversion of the coefficients matrix associated with the resulting system of coupled, complex algebraic equations. Calculations have been done for some model conservative gases and results are presented in Chapter 9. In particular, the effects of the magnetic field strength and angle between the electric and magnetic fields on the spatial relaxation process of electrons are discussed.

4.2.1 Boundary conditions

In this thesis we apply the similar boundary conditions as in recently works of Li (2002; 2006). At the \( z = z_0 \) plane, a disturbing source is applied to charged-particle distribution functions via a drifted Maxwellian velocity distribution:

\[
f_{DM}(c) = A \left( \frac{m}{2\pi kT_i} \right)^{3/2} \exp \left[ -\frac{m(c - v_i)^2}{2kT_i} \right],
\]

(4.11)

where \( v_i \) and \( T_i \) are prescribed drift velocity and temperature parameters, respectively, while the parameter \( A \) is the normalization factor. The boundary conditions at the \( z = z_0 \) plane are on the odd spherical harmonics projections and in terms of the moments of the distribution function we have:

\[
F(\nu lm; \alpha, z_0) = F(\nu lm) \quad (l = 1, 3, \ldots).
\]

(4.12)

In the asymptotic region far downstream from \( z = z_0 \), the distribution function becomes spatially independent and since we consider conservative collisional processes only we have:

\[
\frac{\partial}{\partial z} F(\nu lm; \alpha, z_{\text{max}}) = 0 \quad (l = 0, 2, \ldots),
\]

(4.13)

where \( z_{\text{max}} \) denotes the upper boundary. As already remarked by Li (1999), the boundary conditions proposed above yield stable and physical solutions. Similar but not identical boundary conditions were imposed by Petrov and Winkler (1997) in their method for solving the electron Boltzmann equation in spatially inhomogeneous steady-state plasmas.
4.2.2 Treatment of spatial derivatives using pseudo-spectral and finite difference methods

In this section we apply pseudo-spectral and finite difference method to numerically solve the system of coupled differential equations (3.70) with the boundary conditions (4.12) and (4.13). It should be emphasized once more that we consider the basis temperature $T_b$ as a space-independent constant. This stands in contrast with respect to the time-dependent hydrodynamic problem where a self-consistent method for the determination of $T_b$ has been developed and relatively easy implemented (see Section 5.4). Solution of the boundary value problem discussed here with a space-dependent basis temperature $T_b(z)$ is a laborious task, unless $T_b(z)$ can be somehow specified before numerical solution proceeds (Li et al., 2002). In addition, matrix elements of the collision operators, which depend on basis temperature, would have to be calculated and stored for all spatial mesh points, which is computationally expensive in both time and memory. Hence as already remarked, we follow the prescription proposed by Li (1999) and (Li et al., 2002): the basis temperature $T_b$ is independent of position and high order Sonine polynomial expansion procedure is employed in order to compensate for such a drawback.

Before discussing the pseudo-spectral and finite difference method that has been applied in this work, it should be noted that we have also considered the numerical method proposed by Li et al. (2002; 2006). In their previous work (Robson et al., 2000), an eigenvalue theory of the spatially inhomogeneous Boltzmann equation was developed and applied to study the spatial relaxation of a non-hydrodynamic electron swarm in an idealized SST experiment, under a spatially uniform electrostatic electric field. Very recently, however, their eigenvalue theory was generalized to include both electric and magnetic fields which are orthogonal to each other. Such generalized eigenvalue theory was then employed to study the spatial relaxation of the electrons for a range of model and real gases (Li et al. (2006)). In addition, in the same reference they employ similar technique for solving the Boltzmann equation when both electric and magnetic fields are present as for the electric field only case. A finite difference method was used to treat the spatial dependencies and consequently the Boltzmann equation was converted to a sparse, block, quasi-tri-diagonal system of algebraic equations for the moments of the distribution function. The resulting system of algebraic equation was tackled via the partition scheme initially developed by Li (1999). It is our opinion however, that the proposed numerical scheme for solving the Boltzmann equation cannot be applied when both the electric and magnetic fields are present, independently of the field configuration. When both electric and magnetic field are present, due to the introduction of the additional $m$ index, some of the block matrices associated with the reduced matrix elements of the velocity derivative introduced within the partition scheme of Li (1999) are singular and cannot be inverted. Thus the partition scheme developed by Li (1999) will generally fail if both electric and magnetic fields are present. In this work we employ both the pseudo-spectral and finite difference method to treat the spatial dependence of the distribution function and its moments.

The system of coupled differential equations (3.70) with the boundary conditions (4.12) and (4.13) is solved by approximating the derivative term by some numerical scheme and converting
the system of differential equations into a system of algebraic equations. In general the derivative at a point \( z = z_i \) is represented generally as:

\[
\frac{\partial}{\partial z} F(\tilde{\nu}'; \alpha, z) = \sum_{j=1}^{N} D_{ij} F(\tilde{\nu}'; \alpha, z_j),
\]

where the form \( D_{ij} \) determines the numerical scheme to be implemented. In this work we use two different forms of the \( D_{ij} \): (i) from discrete ordinate; and (ii) from finite differencing.

4.2.2.1 Pseudo-spectral method

In this section we apply the Discrete Ordinate (DO) method which falls into the category of the methods of Weighted Residuals. The DO method or the so-called Pseudo-spectral method was developed initially by Wick (Williams, 1971) as a technique to solve the integral equations. As a practical tool, this method was developed by Chandrasekhar (1960) who used it solve the radiative transfer problem. Application of the DO method to kinetic theory was initiated by Shizgal and co-workers (Shizgal and MacMahon (1985); MacMahon and Shizgal (1985)). Considerable contribution has been made by Robson and co-workers (Robson et al. (1991); Robson and Prytz (1993)) and by White (1993).

To apply the pseudo-spectral method to (3.70), we need to approximate the unknown moments \( F(\tilde{\nu}'; \alpha, z) \) by a truncated series of the trial functions \( T_j(z) \):

\[
F(\tilde{\nu}'; \alpha, z) \approx \sum_{j=1}^{N} a_j T_j(z_i),
\]

where the summation is over the \( N \) collocation points \( z_j \) and \( T_j(z_i) \) are differentiable and well behaved on the domain. The pseudo-spectral method is designated by trial functions which have the property

\[
T_j(z_i) = \delta_{ij}.
\]

If the trial functions are \((N - 1)^{th}\) order polynomials then they have the form outlined by Robson et al. (1991):

\[
T_i(z) = \prod_{j=1}^{N} \frac{(z - z_j)}{z_i - z_j} \approx \frac{\Phi_N(z)}{(z - z_i) \Phi_N'(z_i)},
\]

where \( \Phi_N \) is an \( N^{th} \) order polynomial with zeros at the collocation points \( z_1, z_2 + \cdots + z_N \). The \( T_i(z) \) in (4.17) are referred to as Lagrange polynomials. The error associated with (4.15) is given by

\[
R_N(z) = \frac{f^{(N)}(\zeta)}{k_N N!} \prod_{j=1}^{N} (z - z_j),
\]

where \( z_0 < \zeta < z_N \) and \( k_N \) is the leading coefficient of \( z^N \) in \( \Phi \). That is, (4.15) is exact if the moment \( F(\nu'; \alpha, z) \) is a polynomial of degree \( N - 1 \), or less. Substitution of (4.16) into (4.15)
yields at the collocation points $z_j$

$$F(\tilde{\nu}', \alpha, z) \approx \sum_{j=1}^{N} a_j T_j(z_i)$$

$$= \sum_{j=1}^{N} a_j \delta_{ij}$$

$$= a_i .$$  \hspace{1cm} (4.20)

Thus the coefficients in the expansion (4.15) are the moments evaluated at the collocation points and we have forced approximation (4.15) to be exact at the collocation points. Therefore, we have

$$F(\tilde{\nu}', \alpha, z) = \sum_{j=1}^{N} F(\tilde{\nu}', \alpha, z_j) T_j(z_i) .$$  \hspace{1cm} (4.21)

This equation allows us to express the derivative terms in the matrix representation:

$$\frac{\partial}{\partial z} F(\tilde{\nu}', \alpha, z) = \sum_{j=1}^{N} F(\tilde{\nu}', \alpha, z_j) \frac{\partial}{\partial z} T_j(z)$$

$$= \sum_{j=1}^{N} D_{ij} F(\tilde{\nu}', \alpha, z_j) ,$$  \hspace{1cm} (4.22)

where $D_{ij}$ is the matrix representation of the derivative operator given by

$$D_{ij} = \begin{cases} \frac{\Phi'(z_i)}{(z_i - z_j)\Phi_N'(z_j)} & \text{for } i \neq j \\ \frac{\Phi''(z_i)}{2\Phi_N'(z_j)} & \text{for } i = j. \end{cases}$$  \hspace{1cm} (4.23)

Using (4.16), the first derivative matrix can be represented by

$$D_{ij} = \begin{cases} \frac{1}{(z_j - z_i)} \prod_{k \neq i}^{N} (z_i - z_k) & \text{for } i \neq j \\ \sum_{k \neq i}^{N} (z_i - z_k)^{-1} & \text{for } i = j. \end{cases}$$  \hspace{1cm} (4.24)

Substitution of (4.21) and (4.22) into (3.70) yields:

$$\sum_{j=1}^{N} \sum_{\nu'} [\tilde{p}_{\tilde{\nu},\tilde{\nu}'} \delta_{ij} + \tilde{q}_{\tilde{\nu},\tilde{\nu}'} D_{ij}] F(\tilde{\nu}', \alpha, z_j) = 0 .$$  \hspace{1cm} (4.26)

where

$$\tilde{p}_{\tilde{\nu},\tilde{\nu}'} = \left\{ n_0 l_{\nu'}^{l'}(\alpha) \delta_{\nu'\nu'} \delta_{mm'} + i\alpha(l'm10|lm) < \nu l|l'K^{[1]}|l' > \delta_{mm'} \\
+ \Omega \left\{ \frac{\sin \Psi}{2} \left[ \sqrt{(l-m)(l+m+1)} \delta_{m'm+1} - \sqrt{(l+m)(l-m+1)} \delta_{m'm-1} \right] \\
- i m \cos \Psi \delta_{mm'} \right\} \delta_{\nu'} \right\}$$  \hspace{1cm} (4.27)

$$\tilde{q}_{\tilde{\nu},\tilde{\nu}'} = -\frac{1}{\alpha} (l'm10|lm) < \nu l|\alpha c^{[1]}|l' > \delta_{mm'} \delta_{\nu'\nu'}$$  \hspace{1cm} (4.28)
Therefore, the system of coupled differential equations (3.70) reduces to the solution of the matrix equation (4.26). This matrix equation has the following form:

\[
\begin{bmatrix}
\tilde{p}_{\tilde{\nu}, \tilde{\nu}} D_{11} & \tilde{q}_{\tilde{\nu}, \tilde{\nu}} D_{12} & \cdots & \cdots \\
\tilde{q}_{\tilde{\nu}, \tilde{\nu}} D_{21} & \tilde{p}_{\tilde{\nu}, \tilde{\nu}} D_{22} & \cdots & \cdots \\
\vdots & \vdots & \ddots & \vdots \\
\tilde{q}_{\tilde{\nu}, \tilde{\nu}} D_{N1} & \cdots & \cdots & \tilde{p}_{\tilde{\nu}, \tilde{\nu}} D_{NN}
\end{bmatrix}
\begin{bmatrix}
F_0(\tilde{\nu}; \alpha) \\
F_1(\tilde{\nu}; \alpha) \\
\vdots \\
F_N(\tilde{\nu}; \alpha)
\end{bmatrix} = \begin{bmatrix} 0 \\
0 \\
\vdots \\
0 \end{bmatrix}
\]

Note that the boundary conditions (4.12) and (4.13) associated with (3.70) must also be discretized at the collocation points. Since our problem is a typical two-boundary value problem, we collocate at the \(N - 2\) interior collocation points using (4.20) leaving the first and \(N^{th}\) rows for the discretized boundary conditions. Concerning the structure of collocation points, it should be noted that the pseudo-spectral method places no restriction on the location of the collocation points. Calculations have been done using the uniformly spaced collocation points and roots of Laguerre polynomials. In particular, the Laguerre collocation points were initially chosen since their domain \([0, \infty)\) corresponded to the domain on which the problem is solved. These collocation points are crowded near the origin and increase in spacing as we move away from the origin. The roots of Laguerre polynomials were calculated using a public domain numerical routine published in the second edition of *Numerical Recipes in Fortran 77* (Press et al., 1992).

The first preliminary calculations have been done for some model gases using a small number of collocation points (up to \(N = 50\)). The unknown spatially dependent moments are determined via direct numerical inversion of the coefficient matrix (4.29). An excellent agreement between the numerical solutions of the Boltzmann equation and Monte Carlo results for the steady-state transport properties was found. This validates our strategy for numerically solving the system of coupled differential equations (3.70), implementation and choice of boundary conditions and numerical integrity of our computer code. However, if slow oscillatory relaxation profiles of the spatially resolve transport properties are developed, then the number of collocation points \(N\) must be significantly increased. This fact has introduced new difficulties mainly associated with the memory resources of our computers used for numerical computations. Usually the coefficient matrix (4.29) is very large. The number of non-zero elements \(N_z\) within the coefficient matrix (4.29) is given by

\[
N_z = N(4\nu^2 + 8\nu - 4) + 4n_z(n_z - 1)(\nu - 1) .
\]

Therefore, under the traditional two-term approximation, \(l_{\text{max}} = 1\), assuming typical values \(\nu_{\text{max}} = 65\) and \(N = 1000\) the number of non-zero elements within the coefficient matrix is 260485000. Solving this large system of equations using a double precision for the variables require approximately 8 Gb of the RAM for addressing the non-zero elements and approximately 2 Gb of RAM for their indexing. It is obvious that the pseudo-spectral method suffers from a problem of insufficient storage space at the modern desktop computers. In what follows we present an efficient method to deal with this problem.
4.2.2.2 Finite difference approximation

As observed by Li et al. (2002; 2006), the application of the finite-difference method for a treatment of spatial dependencies converts the system of coupled differential equations (3.70) into a sparse, block, quasi-tri-diagonal system of algebraic equations for the unknown moments. With the feasibility for solving tri-diagonal equations in mind via direct numerical inversion of the coefficient matrix, the derivative operator $D_{ij}$ is modified and coded directly into the program. In these modifications a second order finite difference scheme is assumed for numerical differentiation. The numerical differentiation involve equally-spaced abscissas $z_i$, i.e., a mesh generated by

$$z_i = z_{i-1} + h \quad i = 1, 2, \ldots, N - 1 ,$$

(4.31)

where $h$ is the step size. Forward and backward differencing methods are used at the lower and upper boundaries respectively, while central differencing is used in the intermediate regions. If $g_i$ denote the corresponding ordinates, then for the central difference formula we have

$$(Dg)_i \left( \frac{g}{z} \right)_{z=z_i} = \frac{g_{i+1} - g_{i-1}}{2h} + O \left( h^2 \right) ,$$

(4.32)

or, in general

$$(Dg)_i = \sum_{j=0}^{N-1} D_{ij} g_j + E_i^{(N)} ,$$

(4.33)

where $D_{ij}$ denotes the appropriate matrix representation and $E_i^{(N)}$ is an error term. For the central differencing method, the matrix representation of the derivative operator is given by:

$$D_{ij} = \frac{1}{2h} (\delta_{j,i+1} - \delta_{j,i-1}) .$$

(4.34)

Similarly, the matrix representation of the forward differencing method is given by

$$D_{ij} = \frac{1}{2h} (-\delta_{j,i+2} + 4\delta_{j,i+1} - 3\delta_{ij}) ,$$

(4.35)

while for the backward differencing method one has

$$D_{ij} = \frac{1}{2h} (3\delta_{ij} - 4\delta_{j,i-1} + \delta_{j,i+2}) .$$

(4.36)

Application of the derivative operators (4.34)-(4.36) and applying the boundary conditions (4.12) and (4.13), the system of coupled differential equations (3.70) is converted to sparse, block, quasi-tri-diagonal system of algebraic equations for the unknown moments $F(\tilde{\nu}; \alpha, z)$:

$$
\begin{bmatrix}
C_a & D_a & E_a \\
-D & C & D \\
-D & C & D \\
\ddots & \ddots & \ddots \\
-D & C & D \\
E_b & D_b & C_b
\end{bmatrix}
\begin{bmatrix}
F_0(\tilde{\nu}; \alpha) \\
F_1(\tilde{\nu}; \alpha) \\
F_2(\tilde{\nu}; \alpha) \\
\vdots \\
F_{N-2}(\tilde{\nu}; \alpha) \\
F_{N-1}(\tilde{\nu}; \alpha) \\
F_N(\tilde{\nu}; \alpha)
\end{bmatrix}
= 
\begin{bmatrix}
U \\
0 \\
0 \\
\vdots \\
0 \\
0 \\
0
\end{bmatrix}
$$

(4.37)
where the block matrices $C_a, D_a, \ldots, D_b, E_b$ and block vectors $F_0, F_1, F_N$ and $U$ are dimensioned by $n \times n$ and $n$ respectively, and $n$ is given by $n = (l_{\text{max}} + 1)(\nu_{\text{max}} + 1)$ while $n_z + 1$ is the number of discrete spatial mesh points. The elements of these matrices are:

\[
(C_a)_{\tilde{\nu}, \tilde{\nu}'} = \begin{cases} 
3 \delta_{\nu \nu'} \delta_{ll'} \delta_{mm'} & l = \text{even} \\
2h \tilde{p}_{\tilde{\nu}, \tilde{\nu}'} + 3 \tilde{q}_{\tilde{\nu}, \tilde{\nu}'} & l = \text{odd}
\end{cases} \tag{4.43}
\]

\[
(D_a)_{\tilde{\nu}, \tilde{\nu}'} = \begin{cases} 
4 \delta_{\nu \nu'} \delta_{ll'} \delta_{mm'} & l = \text{even} \\
4 \tilde{q}_{\tilde{\nu}, \tilde{\nu}'} & l = \text{odd}
\end{cases} \tag{4.44}
\]

\[
(E_a)_{\tilde{\nu}, \tilde{\nu}'} = \begin{cases} 
-\delta_{\nu \nu'} \delta_{ll'} & l = \text{even} \\
-\tilde{q}_{\tilde{\nu}, \tilde{\nu}'} & l = \text{odd}
\end{cases} \tag{4.45}
\]

There are many different techniques which can be used to solve the large matrix equation (4.37). In this thesis, the large system of complex algebraic equations is solved by direct inversion of the left hand side. Following the strategy developed under hydrodynamic conditions, in the present code the sparseness of the coefficient matrix is exploited using a public domain Y12M system of sparse matrix inversion routines (Zlatev et al., 1981). It should be noted, however, that this method suffers from a problem of insufficient storage space, even at the modern desktop computers. When the relaxation characteristics are slow and oscillatory, the number of mesh points must be increased. As a consequence, the dimension of this matrix equation is significantly enlarged and in general under these conditions the code usually fails.

Having in mind the limitations and restrictions associated with the method based on the direct inversion of the coefficient matrix, we propose another technique which can be used. This method is based on a Gaussian elimination with backsubstitution. This method reduces a matrix not all the way to the identity matrix, but only halfway, to a matrix whose components on the
diagonal and above remain non-trivial. Thus the matrix equation (4.37) reduces to

\[
\begin{bmatrix}
A_1 \quad D_a \quad E_a \quad 0 \quad 0 \quad 0 \quad \ldots \quad 0 \quad 0 \\
0 \quad A_2 \quad B_2 \quad 0 \quad 0 \quad 0 \quad \ldots \quad 0 \quad 0 \\
0 \quad 0 \quad A_3 \quad D \quad 0 \quad 0 \quad \ldots \quad 0 \quad 0 \\
0 \quad 0 \quad 0 \quad A_4 \quad D \quad 0 \quad \ldots \quad 0 \quad 0 \\
0 \quad 0 \quad 0 \quad 0 \quad A_5 \quad D \quad \ldots \quad 0 \quad 0 \\
\vdots \quad \vdots \quad \vdots \quad \vdots \quad \vdots \quad \vdots \quad \ddots \quad \vdots \quad \vdots \\
0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad \ldots \quad A_{N-1} \quad D \\
0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad \ldots \quad 0 \quad A_b
\end{bmatrix}
\begin{bmatrix}
F_0(\tilde{\nu};\alpha) \\
F_1(\tilde{\nu};\alpha) \\
F_2(\tilde{\nu};\alpha) \\
F_3(\tilde{\nu};\alpha) \\
F_4(\tilde{\nu};\alpha) \\
\vdots \\
F_{N-1}(\tilde{\nu};\alpha) \\
F_N(\tilde{\nu};\alpha)
\end{bmatrix}
= 
\begin{bmatrix}
U_1 \\
U_2 \\
U_3 \\
U_4 \\
U_5 \\
\vdots \\
U_{N-1} \\
U_N
\end{bmatrix}
\] (4.46)

For \( n_z < 4 \), expressions for the block matrices \( A_1, A_2 \) and \( A_3 \) are given as follows:

\[
A_1 = C_a, \\
A_2 = C + D C_a^{-1} D_a, \\
A_3 = C + D A_2^{-1} B_2, 
\] (4.47)

where

\[
B_2 = D + D C_a^{-1} E_a. 
\] (4.48)

The block matrix \( A_n \) for \( 4 \leq n \leq N - 1 \) is given by

\[
A_n = C + D A_{n-1}^{-1} D, 
\] (4.49)

while the block matrix \( A_b \) is given by

\[
A_b = C_b - (D_b - E_b A_{N-2}^{-1} D) A_{N-1}^{-1} D 
\] (4.50)

For the block vectors \( U_1, \ldots, U_{n_z} \) we have

\[
U_1 = U \\
U_n = D A_{n-1}^{-1} U_{n-1}, \quad 2 \leq n \leq N - 1 \\
U_N = -E_b A_{N-2}^{-1} U_{N-2} - (D_b - E_b A_{N-2}^{-1} D) A_{N-1}^{-1} U_{N-1}. 
\] (4.51)

We observe that the last unknown moment \( F_{n_z}(\tilde{\nu};\alpha) \) is isolated, namely

\[
F_N(\tilde{\nu};\alpha) = A_b^{-1} U_N. 
\] (4.52)

With the last moment known we can move to the penultimate moment,

\[
F_{N-1}(\tilde{\nu};\alpha) = A_{N-1}^{-1} (U_{N-1} - D F_N(\tilde{\nu};\alpha)), 
\] (4.53)

and then proceed with the moments before that one. The typical step is

\[
F_n(\tilde{\nu};\alpha) = A_n^{-1} (U_n - D F_{n-1}(\tilde{\nu};\alpha)). 
\] (4.54)

The advantage of Gaussian elimination with backsubstitution over direct inversion technique is clearly evident. The large system of coupled complex algebraic equations (4.37) is transformed to a number of small equations given by (4.47)-(4.54) which can be solved by direct method. Note that this method does not suffer from a problem of insufficient storage space and majority of matrices can be stored online. We believe that this method may work efficiently for this problem and defer its implementation for a future work.
4.2.3 Truncation, convergence and choice of basis temperature

There are a number of parameters involved in the numerical solution of the system of equations (4.37) for the problem at hand. These include $\nu, l, m, z, N$ and $T_b$. First, as already emphasized, the basis temperature $T_b$ is regarded as a space-independent quantity in this work. The first step then would be to choose an initial basis temperature which usually corresponds to that used under hydrodynamic conditions. Following the strategy developed under hydrodynamic conditions, the velocity space indices $\nu, l, m$, are truncated independently until some convergence criterion in the transport properties is satisfied. Usually we take an initial value of $\nu_{\text{max}}$ to be that required under hydrodynamic conditions while regarding the $l$ index, we assume $l_{\text{max}} = 1$ as an initial value, i.e. a two-term approximation. Next the value of $N$ is specified and an initial estimate of the upper boundary $z_{\text{max}}$ is made. The value of $z_{\text{max}}$ is then increased until the equilibrium state is reached. If the equilibrium state is reached, the transport properties are then calculated again with an incremented $\nu_{\text{max}}$. If necessary, both $N$ and $z_{\text{max}}$ can be further incremented. The index $l_{\text{max}}$ is then incremented and the whole procedure repeated until convergent results are obtained. If the above convergence criteria cannot be satisfied for the current basis temperature, the scheme for this basis temperature is said to have failed, and another basis temperature must be sought. Similar convergence testing has been used by Li (1999).
Chapter 5

Monte Carlo simulation technique

5.1 Introduction

In the previous chapters we introduced the elements of both hydrodynamic and non-hydrodynamic transport theory of a swarm of charged particles moving in a neutral gas under the influence of both electric and magnetic fields. An alternative approach to the problem is through the Monte Carlo simulation. The Monte Carlo method is an approach to solve the problem of charged particles transport based on the numerical simulation of the motion of a large particle ensemble where the collision processes are introduced by generating appropriately distributed random numbers. This technique is rigorous but yet flexible method for simulating the transport processes of a swarm of charged particles under both the hydrodynamic and non-hydrodynamic conditions. Independently of the nature of charged particles (electrons or ions), this method consists of several important steps. Usually the charged particles are released with a certain energy and direction of motion. The motion of a single charged particle is followed until collision with the background molecule of a neutral gas occurs. The nature of the collision is randomly selected taking into account the ratio of the cross sections for the possible collision processes at that energy. The type of collision determines the scattering parameters after collision including the charged particle speed and direction of the motion. The last step is determination of the transport properties from the characteristics of the charged particles motion. The way of sampling of transport properties is based upon the method of swarm observation.

In this chapter we consider the basic elements of Monte Carlo codes employed in this thesis. The initial version of the Monte Carlo simulation code was developed at the Institute of Physics in Belgrade. The code has been used to treat a variety of physical problems including the studies of negative electron mobility in both dc (Dyatko et al., 2000) and rf fields (Dujko et al., 2003), kinetic phenomena such as anomalous anisotropic diffusion (Maeda et al. (1997); Raspopović et al. (2000)), time resolved negative differential conductivity (Bzenić et al., 1999), benchmarking in dc and rf fields (Raspopović et al., 1999) and in many other important aspects of plasma modeling. In order to cover some particular aspects of this work in the framework of hydrodynamic studies, the initial version of the computer code has been improved by introducing
new elements. In particular, the code has been extended to consider the electron transport under conditions where dc electric and magnetic fields are crossed at an arbitrary angle. The inclusion of an arbitrarily oriented magnetic field with respect to the electric field vector introduces some additional complexity in the electron motion. To facilitate numerical calculation, a large number of the electron orbits were calculated and studied. The numerically calculated trajectories must give accurate positions and we propose the following simple test: in the absence of electric field the electron trajectory must be closed circle. The further extensions of a Monte Carlo include the sampling of the spatially resolved characteristics of the electron swarm under an arbitrary field configuration.

A non-trivial extension of the Monte Carlo code to consider the spatial relaxation of the electrons under the influence of both electric and magnetic fields in an idealized steady-state Townsend experiment in the presence of non-conservative collisions was developed. The code is designed to serve as a tool for the fundamental studies associated with the basic mechanisms of the electron spatial relaxation processes. These mechanisms include the different roles of elastic and inelastic collisions, the role of non-conservative collisions and effects of a magnetic field. In particular, the modeling of the Franck-Hertz experiment from the kinetic theory point of view can greatly benefit from these studies. Another possible application of the code is connected more with the plasma modeling. For example, the problem of spatial non-locality in the electron transport in the neighborhood of sources or boundaries can be investigated. In addition to spatially uniform fields, it should be emphasized that a Monte Carlo code developed in this thesis can be used under conditions of spatially non-uniform electric and magnetic fields.

A rigorous analysis of the steady-state Townsend experiment in the presence of non-conservative collisions and both electric and magnetic fields is long overdue and in this chapter we take some important steps in this direction. Special attention is paid on the techniques for sampling the spatially resolved transport data in Monte Carlo simulation. The background of these sampling techniques is a rigorous kinetic theory and this is clearly demonstrated in this chapter. A complete and consistent set of equations for conversion between two types of experiments, time of flight (TOF) and steady-state Townsend (SST) is developed. In later chapters, the numerical calculations based on our Monte Carlo code illustrate the distinctions and links between these two types of transport data.

We begin this chapter with an overview of both versions of Monte Carlo code. While the main algorithms of these codes are different, there are some common blocks behind of these codes. These include a random number generator, simulation of a free electron path between the collisions, determining the probability and nature of the collisions and determining the scattering parameters. These blocks and associated numerical procedures are described in great detail. Apart from the main algorithm, these codes can be distinguished by considering the way of sampling of transport properties. Sampling of hydrodynamic transport properties in infinite electron swarms, is well defined for both dc and ac electric fields when non-conservative collisions are operative. However most experiments deal with SST conditions where at any particular point along the discharge there exist electrons originating from the cathode at different times. In
particular, it is difficult to obtain both space and time resolved data under these conditions and hence an important aspect of this thesis is to give an outline of sampling techniques appropriate to SST experiments.

5.2 Overview of the Monte Carlo codes

In the context of hydrodynamic studies, we apply a Monte Carlo simulation code that follows a large number of electrons (typically $10^4 - 10^6$) through a neutral gas under the influence of uniform electric and magnetic fields. The code employs either static or time-dependent fields. It is assumed that an electron swarm develops in an infinite space. At time $t = 0$, electrons are initially released from the origin with the Maxwellian velocity distribution and with the mean kinetic energy of 1 eV. Electrons gain the energy from the external electric field and dissipate it by collisions to the neutral gas molecules. The collisional transfer of this energy to the neutral gas molecules occurs by elastic and different types of inelastic collisions. It is also assumed that the electron density is sufficiently small so Coulomb interactions between the particles as well as shielding of the field is negligible. All calculations were performed for zero gas temperature. In all simulations the gas number density is $3.54 \times 10^{22} \text{ m}^{-3}$ which corresponds to the pressure of 1 Torr at 273 K. Transport coefficients are obtained after the relaxation to the steady-state.

In the context of non-hydrodynamic studies, we apply our steady-state Townsend Monte Carlo simulation code and follow the trajectories of a large number of electrons which undergo collisions with background neutral particles. The primary electrons are isotropically released one by one from the cathode surface into the half space with an initial energy $\epsilon_0$. Any new secondary electrons arising from electron impact ionization events are followed using the following procedure. When an ionization collision occurs, the set of all dynamic properties (the moment of an ionization collision, the position of new electron, the starting energy and velocity) of secondary electron are placed at the stack. When primary electron reaches the anode surface or disappears in an attachment collision event, the first available electron from the stack is followed. These secondary electrons from the stack are released isotropically. In an attachment collision the electron is consumed and hence no simulated further. If the stack is empty, the next primary electron is released and the whole procedure repeats. Thermal motion of the background neutral particles and electron-electron interactions are neglected. The electrodes are considered to be perfectly absorbing.

5.3 Random number generator

One of the most critical components in Monte Carlo simulation is the quality of the pseudo-random number generator. Our codes employ the generator ran3 published by Press et al. (1994) which has been claimed to have a period length of $2^{55} - 1$ and it requires an initializing sequence of 55 numbers. The early development of a code reveals the correlation of the fifth order. The manifestation of this correlation was an unphysical increase of the average coordinate.
of a swarm of the electrons in the $\mathbf{E} \times \mathbf{B}$ direction for a magnetic free field case. The correlation was removed in our codes by separating the random numbers generators. Better random number generators can be found but the penalty is a significant increase in the computation time.

### 5.4 Simulation of an electron path in electric and magnetic fields

In this section we describe in detail how the path of an individual electron in electric and magnetic fields is simulated. The equation of motion of a single electron is determined from the forces acting on the electron. If the forces are due to electric and magnetic fields, the Newton’s second law can be written as

$$m \frac{d\mathbf{v}}{dt} = e \mathbf{E} + ev \times \mathbf{B}, \quad (5.1)$$

where $e$ and $m$ are the charge and mass of the electron, respectively. We now introduce the quantity

$$\Omega = \frac{eB}{m}. \quad (5.2)$$

This is the cyclotron frequency of gyration of the electron about the magnetic field lines. We employ a coordinate system where $\mathbf{E}$ defines the $x$-axis while $\mathbf{B}$ lies in the $x$-$z$ plane making an angle $\varphi$ with respect to the $\mathbf{E}$. Then (5.1) can be written in scalar form as

$$\frac{dv_x}{dt} = \left( \frac{e}{m} E + \Omega v_y \sin \varphi \right)$$

$$\frac{dv_y}{dt} = (\Omega (v_z \cos \varphi - v_x \sin \varphi))$$

$$\frac{dv_z}{dt} = -\Omega v_y \cos \varphi, \quad (5.3)$$

from which we obtain the analytical solutions for the velocity and displacement components of the electron. Similar but not identical explicit form of analytical solutions is given elsewhere (Biagi, 1999) and according to these equation the motion of a single electron through the neutral gas is followed between collisions.

Another technique widely used in plasma physics for the determination of the electron motion is the 'Boris rotation', which is a form of predictor-corrector scheme (Birdsall and Langdon, 1974). This technique is employed in our Monte Carlo code when electric and magnetic fields are assumed to be time-dependent. In such a case the magnetic field is oriented along the $z$ axis. It is important to emphasized that this technique cannot be applied for an arbitrary configuration of the fields. Boris rotation algorithm is based on the use of the electric field only. After each time step used for a movement of electron ($\Delta t$), the electron velocity is rotated in such a way as to obtain the effect of a magnetic field. The angle of rotation is dependent on the magnitude of the magnetic field. According to this procedure, the additional velocities were introduced

$$v'_x = v_x + \tan \left( -\frac{\theta}{2} \right) v_y \quad (5.4)$$

$$v'_y = v_y - \tan \left( -\frac{\theta}{2} \right) v_x \quad (5.5)$$
where \( v_x \) and \( v_y \) are the current components of the electron velocity with a time step of \( \Delta t/2 \). The angle of rotation, \( \theta \) is given by
\[
\theta = \frac{eB}{m} \Delta t .
\] (5.6)

Since the magnetic field is oriented along the \( z \) axis, the new components of the drift velocities are obtained by the following rotation
\[
v_x = v_x + sv_y',
\] (5.7)
\[
v_y = v_y - sv_x',
\] (5.8)
where \( s \) and \( t \) are the parameters of rotation given by
\[
t = -\tan \left( \frac{\theta}{2} \right)
\] (5.9)
\[
s \equiv -\sin \theta = \frac{2t}{1 + t^2}.
\] (5.10)

At the end of this procedure, it is necessary once more to accelerate the electron along the electric field using the time step of \( \Delta t/2 \). The displacement components are given by
\[
x = x_0 + \frac{1}{2} (v_{x0} + v_x(t)) \Delta t ,
\] (5.11)
\[
y = y_0 + \frac{1}{2} (v_{y0} + v_y(t)) \Delta t,
\] (5.12)
\[
z = z_0 + v_z(t) \Delta t ,
\] (5.13)
where \( x_0, y_0 \) and \( z_0 \) are the initial positions.

The last option for the determination of the electron motion in electric and magnetic fields would be the classical finite differential scheme for numerical integration of the equations of electron motion. This method may be expressed as follows
\[
\mathbf{v}(t + \Delta t) = \mathbf{v}(t) + \frac{e}{m} (\mathbf{E} + \mathbf{v}(t) \times \mathbf{B}) \Delta t
\] (5.14)
\[
\mathbf{r}(t + \Delta t) = \mathbf{r}(t) + \mathbf{v}(t) \Delta t .
\] (5.15)

In the limit of an orthogonal field configuration (where magnetic field is oriented along the \( z \) axis) the vector equation (5.14) has the following scalar representation
\[
v_x = v_{x0} + \left( \frac{e}{m} E + \Omega v_{y0} \right) \Delta t
\] (5.16)
\[
v_y = v_{y0} - \Omega v_{z0} \Delta t
\] (5.17)
\[
v_z = v_{z0} ,
\] (5.18)
where \( v_{x0}, v_{y0} \) and \( v_{z0} \) are the initial values of the velocity components. Similarly, from (5.15) we have
\[
x = x_0 + v_{x0} \Delta t
\] (5.19)
\[
y = y_0 + v_{y0} \Delta t
\] (5.20)
\[
z = z_0 + v_{y0} \Delta t ,
\] (5.21)
where \( x_0, y_0 \) and \( z_0 \) are the initial positions.

The validity of the Boris rotation algorithm and scalar equations (5.16)-(5.21) is verified in Fig. 5.1. If one assumes \( \mathbf{E} = 0 \) the electron trajectory must be a closed circle in \( xy \) plane. In Fig. 5.1 we show the comparison between the electron trajectories obtained by different methods mentioned above. The initial electron velocity along the \( x \)-axis is \( v_{x0} = 6 \times 10^5 \) m/s, the time step is set to \( \Delta t = 10^{-13} \) s and the magnetic field strength is \( B = 5 \) gauss. The time step \( \Delta t \) is chosen in such a manner that one gyration consists of 20 time steps. While the application of classical finite differential scheme gives entirely inappropriate electron trajectory, the Boris rotation algorithm provides an accurate trajectory. If the time steps \( \Delta t \) are decreased, the finite differential scheme will increase in accuracy but the penalty is significant increase in computation time.

![Figure 5.1: Comparison between electron orbits in uniform, static magnetic field obtained via different techniques for solving the equation of motion of a single electron.](image)

5.5 Determining the probability and nature of the collisions

The crucial features of a Monte Carlo method are to follow accurately the path of an individual electron and to determine the exact moment and the nature of the next collision. Consider a test electron somewhere within the swarm at a moment \( t = t_0 \). The probability that the electron has no collision before the time \( t \) is given by

\[
P(t) = \exp \left( \int_{t_0}^{t} \nu_T(e(t')) dt' \right),
\]

(5.22)
where $t_0$ is either the time of electron entering into the gas or the time of a previous collision. The time-dependent total collision frequency $\nu_T$ is given by

$$\nu_T = n_0 \sqrt{\frac{2e}{m}} \sum_k \sigma_k(\epsilon) ,$$  \hspace{1cm} (5.23)

where the summation runs over all possible collision types $k$, $\sigma_k$ is the cross section, $\epsilon$ is the electron energy and $n_0$ is the density of the background molecules. The probability density that the collision occurs in the time interval $(t, t + \Delta t)$ is given by

$$p(t)dt = P(t) - P(t + \Delta t) ,$$  \hspace{1cm} (5.24)

and hence the integral equation for the collision probability is given by

$$p(t) = \nu_T(\epsilon(t)) \exp \left( - \int_{t_0}^{t} \nu(\epsilon(t')) dt' \right) .$$  \hspace{1cm} (5.25)

A random collision time $t_c$ may be obtained by equalizing the probability that the random number $\xi_1$ is from the uniform distribution on the interval $(0,1)$ and the probability that a random collision time $t_c$ is on the interval $[t_0, t_c]$ and hence

$$- \ln(1 - \xi_1) = \int_{t_0}^{t_c} \nu_T(\epsilon(t)) dt .$$  \hspace{1cm} (5.26)

Equation (5.26) has no analytical solutions for real gases. There are two methods of solving this equation. The first method is known as null-collision method, initially developed by Skullerud (1968) for simulation of ion motion in gases. This method introduces an imaginary collision type: the null collision, which has no effect whatsoever on the electron. The cross section for the null-collision is chosen to obtain a constant total collision frequency $\nu_{tot}$ given by

$$\nu_{tot} = \max \left( n_0 \sqrt{\frac{2e}{m}} \sum_k \sigma_k(\epsilon) \right) .$$  \hspace{1cm} (5.27)

Using $\nu_{tot}$ instead of $\nu_T(t)$, equation (5.26) reduces to

$$t_c = t_0 - \frac{1}{\nu_{tot}} \ln(1 - \xi_1) .$$  \hspace{1cm} (5.28)

The null-collision method has been used extensively for electron swarms under both the hydrodynamic (for example, see Brennan et al. (1990); Brennan (1991); White et al. (1997) and Longo (2000)) and non-hydrodynamic conditions (Kortshagen et al. (1996a) and Stojanović and Petrović (1998)). In order to improve the speed of the codes, the different energy regions associated with the different null-collision cross sections may be introduced. Such a technique has been firstly developed by Reid (1977) and it is of a particular interest when null-collisions dominate the real collisions.

However, the null-collision technique does not have an advantage for time-dependent fields as the procedure has to be stopped many times during one field period in order to change the electric and/or magnetic fields. Thus, we employ the integration method, which is based on
numerical integration of the equation (5.26). According to this method, the equation (5.26) may be written as

\[ \ln(1 - \xi_1) \leq \sum_i \nu_T(\epsilon(t_i))\Delta t_i . \]  

(5.29)

The sum of the inequality (5.29) is usually known as the collision sum. The essence of this method is to check whether the collision sum becomes greater than the logarithm of a random number. If an equality (5.29) does not hold for some \( \Delta t_k \), the collisions occurs and \( \sum \Delta t_k \) represents the solution.

It is obvious that the most critical step of the integration method is to decide how long the time-steps for numerical integration should be. In our code the time steps are determined as the minimum of the three relevant time constants (mean collisions time, cyclotron period for \( E \times B \) and period of the field) divided by a large number. Varying the number that is used to divide the time constants gives a test of the convergence of the method itself.

Once the moment of the next collision is established, the nature of the collision \( k \) is determined from another uniformly distributed random number \( \xi_2 \) between 0 and 1, taking into account the relative probabilities of the various collision types:

\[ \sum_{j=1}^{k-1} P_j < \xi_2 < \sum_{j=1}^k P_j , \]

(5.30)

where \( P_j \) denotes the partial probabilities given by the ratio of an individual cross section and total cross section at the current electron energy

\[ P_j = \frac{\sigma_j(\epsilon)}{\sigma_T(\epsilon)} . \]

(5.31)

If the null-collision technique is employed to find \( t_c \), one of the possible collision types in equations (5.30) and (5.31) is the null collision.

### 5.6 Determining the scattering parameters

The next step in our Monte Carlo method is to calculate the properties of the electron after the scattering. The change in the direction of the electron velocity is described by an azimuthal angle \( \varphi \) and by the scattering angle \( \theta \). The azimuthal angle is assumed to be uniformly distributed in the range \([0, 2\pi]\)

\[ \varphi = 2\pi \xi_3 , \]

(5.32)

where \( \xi_3 \) is a new uniformly distributed random number between 0 and 1. The scattering angle may be anisotropically distributed and the probability for the electron with energy \( \epsilon \) to be scattered over an angle \( \theta \) is determined by the differential cross section \( I(\epsilon, \theta) \). In this thesis we assume that all electron scattering are isotropic regardless of the collision nature, thus a random scattering angle \( \theta \) may be found simply as:

\[ \theta = \arccos(1 - 2\xi_4) . \]

(5.33)
In case of isotropic scattering, the elastic collision frequency should be calculated using the momentum transfer cross section instead of the total elastic cross section. It must be emphasized that this approximation is generally valid for relatively low $E/n_0$ but needs to be corrected when forward scattering becomes dominant. In that respect, Biagi (1999) has adopted the method proposed by Longo and Capitelli (1993) in his Monte Carlo code to include the angular distribution of both elastic and inelastic collisions.

In addition to changing the direction of the electron velocity, the collision affects the electron energy. For elastic collisions, the electron energy after the collision is given by

$$\epsilon_1 = \epsilon \left[ 1 - 2m/M(1 - \cos \theta) \right], \quad (5.34)$$

where $\epsilon$ is the electron energy before the collision, $m$ and $M$ are the electron and neutral molecule masses, respectively. The electron energy after an inelastic collision is simply

$$\epsilon_1 = \epsilon - \epsilon_l , \quad (5.35)$$

where $\epsilon_l$ is the energy loss of an inelastic collision.

When non-conservative collisions attachment and/or ionization are operative, we increase and/or decrease the number of electrons as certain limits are reached. In case of ionization, these limits are associated with the allocation of the computer memory. On the other hand, whenever electron is lost due to attachment another electron is randomly selected in its place from the ensemble of the remaining electrons. By doing so, we compensate the losses due to attachment while not changing the distribution function. The statistical uncertainty of a Monte Carlo simulation decreases inversely with the square root of the number of electrons processed, and hence it is important to retain a relatively large number of electrons in simulation allowing an improvement in statistics.

In case of ionization, the remaining electron energy is redistributed between the primary and the secondary electron. One may use an approximation that the primary electron takes the whole energy while the secondary starts the motion with zero or the semi-empirical formula initially published by Opal and co-workers (Opal et al., 1971). Nevertheless, we adopt a concept where the energy of the primary and secondary electron is determined by introducing the new uniformly distributed random number between 0 and 1, which was shown to be sufficiently accurate in our conditions.

## 5.7 Sampling techniques under hydrodynamic and non-hydrodynamic conditions

### 5.7.1 General considerations: distribution functions, macroscopic quantities and hydrodynamic regime

In this section we present our sampling techniques for the electron transport properties under hydrodynamic and SST conditions. The behavior of a swarm of electrons in gases under the
influence of electric and magnetic fields can be described by the time evolution of the phase-space distribution function $f(r, v, t)$ where $r$ and $v$ define co-ordinates in position and velocity space respectively. The phase-space distribution function is defined such that $f(r, v, t)\, dr\, dv$ is the number of particles within $dr$ of $r$ and $dv$ of $v$ at time $t$. The phase-space distribution function can be determined from solution of the Boltzmann equation or from a Monte Carlo simulation. Quantities of interest can be determined from the appropriate integrals over velocity and/or configuration space. For example, the average value of the property $\varphi$ at a given position is defined as:

$$\langle \varphi \rangle = \frac{\int \varphi f(r, v, t)\, dv}{\int f(r, v, t)\, dv} = \frac{1}{n(r, t)} \int \varphi f(r, v, t)\, dv,$$

where $n(r, t)$ is the number density at that position. The mean value of the same property over the entire swarm is

$$\bar{\varphi} = \frac{\int \varphi f(r, v, t)\, dr\, dv}{\int f(r, v, t)\, dr\, dv} = \frac{1}{N} \int \varphi f(r, v, t)\, dr\, dv,$$

where $N$ is the total number of swarm particles.

We are following the conventional definitions of transport coefficients and assume that the hydrodynamic approximation pertains, so that all space-time dependence is expressible through linear functionals of $n(r, t)$ (Kumar et al., 1980). A sufficient representation is a density gradient expansion of the phase-space distribution function (Kumar et al., 1980):

$$f(r, v, t) = \sum_{s=0}^{\infty} f^{(s)}(v) \otimes (-\nabla)^{(s)} n(r, t),$$

where the following normalization condition is satisfied

$$\int f^{(s)}(v)\, dv = \delta_{s0}. \quad (5.39)$$

Substitution of (5.38) into (5.36), yields the density gradient expansion of $\langle \varphi \rangle(r, t)$. The density gradient expansion of the average energy and average velocity are

$$\varepsilon(r, t) = \sum_{s=0}^{\infty} \varepsilon_s (-\nabla)^s n = \bar{\varepsilon} + \gamma \cdot \nabla n + \ldots,$$

$$v(r, t) = \sum_{s=0}^{\infty} \Gamma_s (-\nabla)^s n = W^{(s)} - \frac{1}{n} D^{(s)} \cdot \nabla n + \ldots,$$

where

$$\varepsilon_s = \int \frac{1}{2} m v^2 f^{(s)}(v)\, dv,$$

$$\Gamma_s = \int v f^{(s)}(v)\, dv.$$

Here $\bar{\varepsilon}$ is the mean energy and $\gamma = n \varepsilon_1$ is the gradient energy parameter White et al. (1995), $W^{(s)}$ and $D^{(s)}$ define, respectively, the flux drift velocity and flux diffusion tensor.
5.7.2 The calculation of bulk and flux transport coefficients

In Monte Carlo simulation, the bulk transport coefficients may be determined from the rate of changes of the appropriate averages of the positions of the electron swarm particles, in the real space. The number changing reaction rate is defined by

\[ \omega^{(0)} = -\alpha = \frac{d}{dt} (\ln N), \]  
(5.44)

the drift velocity by

\[ \omega^{(1)} = W(t) = \frac{d}{dt} \langle r \rangle, \]  
(5.45)

and the diffusion tensor by

\[ \omega^{(2)} = D = \frac{1}{2} \frac{d}{dt} \langle r^* r^* \rangle, \]  
(5.46)

where \( N \) is the total number of electrons at any time and \( r^* = r - \langle r \rangle \).

In order to use Monte Carlo simulation to determine the flux transport coefficients one may use approach proposed by Nolan et al. (1997). They have developed the explicit formulas involving distribution functions for the correction terms \( S^{(j)} \) \((j = 0, 1, 2, \ldots)\) which allow the determination of the flux transport coefficients using (2.29) and (2.30). This method requires numerical integration and hence the accuracy of the flux transport coefficients may be affected by the choice of numerical procedure. One may avoid these difficulties using the following simple formulas for the flux drift velocity and flux diffusion tensor components (Petrović et al. (2002); Dujko et al. (2005; 2006)):

\[ W^{(\ast)}(t) = \left\langle \frac{dr}{dt} \right\rangle = \langle v \rangle, \]  
(5.47)

\[ D_{ii}^{(\ast)}(t) = \langle r_i v_i \rangle - \langle r_i \rangle \langle v_i \rangle, \]  
(5.48)

where \( v \) is the electron velocity and \( i = x, y, z \). We shall show below that the procedures adopted by Nolan et al. (1997) and the above formulas are equivalent. It follows from (5.47) that the flux drift velocity is the mean velocity of the electrons. Formulas (5.44)-(5.48) enable direct calculation of both sets of transport coefficients, flux and bulk, in Monte Carlo simulation. Note that the angular brackets denote the averages over all electrons at any moment \( t \). When the hydrodynamic regime is reached, the averages obtained in such a way are independent of time.

In case of time-dependent fields, the results for transport properties are averaged over several periods (phase to phase matched) in order to improve the statistics of the output data.

Both sets of transport properties/coefficients, flux and bulk, are necessary as input data in plasma modeling. The bulk values should be used for the analysis of the validity of the cross section. On the other hand, the flux values should be calculated using the Boltzmann equation or Monte Carlo simulation and then used as input data in fluid modeling of plasma discharges Robson et al. (2005). However, the distinction between these two sets of transport coefficients has often been ignored in previous work in the plasma modeling community (Robson et al., 2005). This has lead to a potentially serious mismatch between input swarm data required and used. Note that only the Boltzmann equation analysis and/or Monte Carlo simulation can
resolve any such mismatch, by providing both flux and bulk transport coefficients. A review of these aspects is contained in reference Robson et al. (2005).

In order to sample spatially resolved transport parameters under hydrodynamic conditions, we have restricted the space and divided it into cells. Every cell contains 100 points and these points are used to sample spatial parameters of electron swarm. This concept of our code allowed us to follow the development of the swarm in both real space and normalized to $6\sigma$, where $\sigma$ is the standard deviation of the Gaussian distribution in space. The spatially resolved electron transport properties including the average energy/velocity have been determined by counting the electrons and their energies/velocities in every cell. Therefore, we may follow the spatial profiles of electron positions as well as spatial profiles of the average energy/velocity as they develop in space and time and within the swarm.

5.7.3 Transport under SST conditions

In this work we study spatial relaxation of the electron transport properties in an idealized steady state Townsend experiment with plane-parallel geometry. A steady stream of electrons emitted from the cathode enters and ionizes the gas and at a sufficiently large distance $z$ from the cathode it is usually assumed that $n(z) \approx \exp(\alpha z)$, where $\alpha$ is the first Townsend ionization coefficient (Boeuf and Marode (1984); Robson (1991); Blevin and Fletcher (1984); Sakai et al. (1977)). In an electron-attaching gas, the electron number density decreases according to the similar exponential law. There exists a steady state in which transport properties are independent of time and vary with the position only. It is generally found that for a region near the cathode/source “non-hydrodynamic” behavior exists (Sakai et al., 1977). In this regime, the continuity equation (2.19) still holds but representations involving low-order density gradient expansions fail (e.g. diffusion equation) and hence concepts of quantities like diffusion coefficients do not necessarily apply in this region. At sufficient distances from the cathode/source, however the velocity dependence (and hence average transport properties) does not vary with position and hydrodynamic conditions prevail.

The transport properties of interest in our SST study are the spatial evolution of the average energy and average velocity. Although we are not advocating the use of labels to assign different transport properties to different experiments, for emphasis in this thesis we shall use the subscript SST to designate that the properties have relaxed to their spatially independent values e.g. “SST average energy” $\varepsilon_{\text{SST}}$ and “SST average velocity” $v_{\text{SST}}$. Assuming the exponential growth of the electron number density with the distance $n(z) \approx \exp(\alpha z)$, it follows from (5.40) and (5.41) that the density gradient expansion of the average energy and average velocity are respectively

$$\varepsilon_{\text{SST}} = \sum_{s=0}^{\infty} \varepsilon_{s}(-\alpha)^{s} = \ddot{\varepsilon} + \gamma \alpha + \ldots ,$$

(5.49)

$$v_{\text{SST}} = \sum_{s=0}^{\infty} \Gamma_{s}(-\alpha)^{s} = W^{(\star)} - D^{(\star)} L \alpha + \ldots ,$$

(5.50)
where \( D_L^{(\ast)} \) is the flux longitudinal diffusion coefficient. From equations (5.49) and (5.50) we can see that the SST average energy and SST average velocity can be calculated from the expansion coefficients, \( \varepsilon_s \) and \( \Gamma_s \) in the density gradient expansions of the average energy and velocity respectively.

It is important to clarify a point which is often a source of confusion introduced in part by terminology. When non-conservative processes are operative, the SST average energy and SST average velocity are different from those determined from hydrodynamic calculations of the mean energy and flux (or bulk) drift velocities respectively (e.g. often calculated in time-of-flight TOF analysis). We shall demonstrate this further in Chapter 9. Rather, \( \varepsilon_{\text{SST}} \) can be calculated from \( \tilde{\varepsilon} \) and \( \gamma \) (plus higher order terms if higher accuracy is required), while \( v_{\text{SST}} \) can be calculated from \( W^{(\ast)} \) and \( D_L^{(\ast)} \) (plus higher order terms if higher accuracy is required). Obviously, in the absence of non-conservative collisions, \( \varepsilon_{\text{SST}} \) reduces to \( \tilde{\varepsilon} \) while \( v_{\text{SST}} \) reduces to \( W^{(\ast)} \).

The present work follows the traditional but rigorous kinetic theory and in that respect strongly supports the conclusions outlined by Robson (1991). Transport coefficients must be independent of the experimental setup from which they were obtained. The true transport coefficients in this sense are the bulk transport coefficients. Other transport “coefficients” (e.g. \( v_{\text{SST}} \)) are dependent on the experimental technique and hence are not strictly speaking true transport coefficients. Likewise, the flux transport properties are not true transport coefficients as they are not measurable but can only be calculated in hydrodynamic calculations.

### 5.7.3.1 Sampling of spatially resolved transport data

Let us consider a swarm of electrons released at time \( t_0 = 0 \) at \( r_0 = 0 \) with a given initial velocity distribution and let \( f(r,v,t) \) be the distribution function of the electrons at time \( t \). Distribution function \( f(r,v,t) \) can be presented as a sum of Dirac’s delta functions:

\[
f(r,v,t) = \sum_{k=1}^{N(t)} \delta(r_k(t) - r) \delta(v_k(t) - v),
\]

where \( N(t) \) is the total numbers of electrons at time \( t \). Integrating \( f(r,v,t) \) over time (from \( t_0 = 0 \) to infinity) we get the steady-state distribution function \( f_{\text{SST}}(r,v) \) which can be written as:

\[
f_{\text{SST}}(r,v) = h \int_0^\infty f(r,v,t)dt = h \sum_{k,l} \frac{1}{v_{zk}(t_l)} \delta(x_k(t_l) - x) \delta(y_k(t_l) - y) \delta(v_k(t_l) - v),
\]

where \( h \) is the flux normalized to 1, \( k \) is the index for all particles of the swarm (from \( t_0 = 0 \) to infinity) and \( l \) is the number of passes of each electron through the plane perpendicular to axis \( z \). Using formula (5.52) one may obtain any physical parameter \( \xi \) of the swarm in SST experiment at the position \( z \) in the following way:

\[
\langle \xi \rangle_z = \frac{\int \xi f_{\text{SST}}(r,v) dx dy dv}{\int f_{\text{SST}}(r,v) dx dy dv}.
\]
This is the so-called “membrane’s sampling” method as it corresponds to passages through a membrane perpendicular to the axis of the electric field. The electron number density, mean energy and average velocity are defined respectively as follows:

\[
n(z) = \int f_{\text{SST}}(r, v) dx dy dv = h \sum_{k,l} \frac{1}{|v_{zk}(t_l)|},
\]

\[
\varepsilon(z) = \left( \sum_{k,l} \frac{1}{|v_{zk}(t_l)|} \right)^{-1} \sum_{k,l} \frac{\varepsilon_k(t_l)}{|v_{zk}(t_l)|},
\]

\[
v_z(z) = \left( \sum_{k,l} \frac{1}{|v_{zk}(t_l)|} \right)^{-1} \sum_{k,l} \frac{v_{zk}(t_l)}{|v_{zk}(t_l)|}.
\]

The second way of sampling is labeled as “sampling in boxes”. According to this method, the abscissa \( z \) is divided into a large number of small boxes \( \Delta z \) wide and infinite over perpendicular axes. Any property may be defined in \( j \)th box (i.e. between \( z_j - \Delta z/2 \) and \( z_j + \Delta z/2 \)) as:

\[
\langle \xi \rangle_j = \left( \frac{1}{\Delta z} \int_{z_j - \Delta z/2}^{z_j + \Delta z/2} f_{\text{SST}}(z, v) dr dv \right)^{-1} \frac{1}{\Delta z} \int_{z_j - \Delta z/2}^{z_j + \Delta z/2} \xi f_{\text{SST}}(z, v) dr dv
\]

\[
\approx \left( \sum_{k=1}^{N} \Delta t^j_k \right)^{-1} \sum_{k=1}^{N} \xi^j_k \Delta t^j_k,
\]

where \( f_{\text{SST}}(z, v) \) is the steady state distribution function, \( \xi^j_k \) is the value of the quantity to be sampled when \( k \)th electron is contained in \( j \)th box, \( \Delta t^j_k \) is the residence time of the electron in that box and \( N \) is the total number of electrons which appear there. Electrons moving towards both the cathode and anode must be considered and sampled. The reasons why the residence time of the electrons must be considered in the above sampling formula are given in Sakai et al. (1972). These two sampling techniques must yield the same results under the same physical conditions in simulation. Both sampling techniques provide spatial variation of transport properties with high spatial resolution. If it is not otherwise specified, in this work the spatially resolved transport properties are obtained via box sampling. The internal consistency between membrane and box sampling has been checked and found to be very good.

The spatially resolved rate coefficients can be calculated by determining the number of collisions of type \( m \) in the \( j \)th spatial box located at \( z_j \) (Stojanović and Petrović, 1998):

\[
\frac{R^m(z_j)}{n_0} = \frac{N^m_j}{\Delta z N_e(z_j)},
\]

where \( N^m_j \) denotes the number of collisions \( m \), \( \Delta z \) is the width of box and \( N_e(z_j) \) represents the net number of residential electrons. This procedure is similar to the actual experimental measurements of spatially resolved excitation and ionization coefficients (Stojanović and Petrović (1998)). Some tests of the procedure have been made by comparing the ionization rate coefficients obtained from the slope of the simulated spatial profile of electron emission and by direct sampling (5.58) with the results produced by integrating the EEDF and the corresponding cross section. In a similar fashion excitation coefficients that may be sampled in the Monte Carlo
simulation at any point may be compared with the integrals of the corresponding cross sections and also compared to the experimental excitation coefficient that may be determined only at the anode. The comparisons of the data obtained from simulations by the two different techniques always gave data that were in good agreement and were an important check of internal consistency especially important if we extend the technique to the non-hydrodynamic situation.

5.7.4 On the calculation of coefficients in the hydrodynamic expansion

One of the questions that concerns us in the present work is the calculation of the expansion coefficients in the density gradient expansion of the transport properties, which are determined from the tensor functions $f^{(s)}(v)$. In order to find these functions we follow the previous works of Kumar et al. (1980), Kumar (1981) and Nolan et al. (1997). We will consider the most general situation, of which the SST case is one limiting case. By doing so, the following tensor functions of rank $k$ may be introduced:

$$N^{(k)} = \int n(r,t) \frac{r^k}{k!} dr = \int F^{(k)}(v) dv,$$

$$F^{(k)}(v) = \int f(r,v) \frac{r^k}{k!} dr.$$  

(5.59)

Although these quantities have clear physical interpretation they cannot be measured in experiments. However, these quantities can be calculated in Monte Carlo simulations. Taking successive moments of the electron number density under SST conditions we have:

$$N^{(0)} = \int n(r,t) dr = \int F^{(0)}(v) dv \equiv N,$$

$$N^{(1)} = \int r n(r,t) dr = \int F^{(1)}(v) dv \equiv N \langle r \rangle,$$

$$N^{(2)} = \frac{1}{2} \int r^2 n(r,t) dr = \int F^{(2)}(v) dv \equiv \frac{1}{2} N \langle rr \rangle,$$

(5.61)  

(5.62)  

(5.63)

where $N$ is the total number of electrons at any time $t$ and the angular brackets denote the averages over all electrons at any moment $t$. Substitution of (5.38) into (5.60) and using (5.61)-(5.63) yield the following expressions for the lowest $F^{(k)}(v)$ tensors:

$$F^{(0)}(v) = N f^{(0)}(v),$$

$$F^{(1)}(v) = N f^{(0)}(v) \langle r \rangle + N f^{(1)}(v),$$

$$F^{(2)}(v) = \frac{1}{2} N \langle rr \rangle f^{(0)}(v) + \frac{1}{2} N \left[ \langle r \rangle f^{(1)}(v) + f^{(1)}(v) \langle r \rangle \right] + N f^{(2)}(v).$$

(5.64)

(5.65)

(5.66)

It is easily seen that, the tensor functions $f^{(s)}(v)$ are given by

$$f^{(0)}(v) = \frac{1}{N} \int f(r,v,t) dr,$$

$$f^{(1)}(v) = \frac{1}{N} \int r f(r,v,t) dr - \frac{1}{N} \int f(r,v,t) dr \frac{1}{N} \int r f(r,v,t) dr dv,$$

(5.67)

(5.68)
\[
f^{(2)}(v) = \frac{1}{2N} \int rrf(r,v,t)dr - \frac{1}{2N} \int rrf(r,v,t)drv \frac{1}{N} \int f(r,v,t)dr \\
- \frac{1}{N} \int rfv(r,v,t)drv \frac{1}{N} \int f(r,v,t)dr + \frac{1}{N} \int f(r,v,t)dr \left[ \frac{1}{N} \int rfv(r,v,t)dr \right]^2.
\]

(5.69)

Under an infinite plane parallel configuration, with the electric field in the \(z\)-direction, the spatial variations are along the \(z\) axis only, with no variations along the \(x\)- or \(y\)-directions.

Substitution of (5.67)-(5.69) into (5.43) allows us to determine the expansion coefficients in the density gradient expansion of the particle flux, or equivalently the flux transport coefficients:

\[
\Gamma_0 = \langle v_z \rangle \equiv W^{(\star)} ,
\]

(5.70)

\[
\Gamma_1 = \langle zv_z \rangle - \langle z \rangle \langle v_z \rangle \equiv D_L^{(\star)} ,
\]

(5.71)

\[
\Gamma_2 = \frac{1}{2} \langle z^2 v_z \rangle - \frac{1}{2} \langle z^2 \rangle \langle v_z \rangle - \langle z \rangle \langle zv_z \rangle + \langle z \rangle^2 \langle v_z \rangle.
\]

(5.72)

Expressions (5.61) and (5.62) independently confirm the validity of using (2.24) in the calculation of the flux drift and flux longitudinal diffusion coefficients. Equation (5.69) allows us to calculate higher order flux terms.

Likewise, substitution of (5.67)-(5.69) into (5.42), respectively, allows us to determine the coefficients in the density gradient expansion of the average energy:

\[
\varepsilon_0 \equiv \tilde{\varepsilon} ,
\]

(5.73)

\[
\varepsilon_1 = \frac{1}{2} \langle z\varepsilon \rangle - \langle z \rangle \langle \varepsilon \rangle \equiv -\frac{\gamma}{n} ,
\]

(5.74)

\[
\varepsilon_2 = \frac{1}{2} \langle z^2 \varepsilon \rangle - \frac{1}{2} \langle z^2 \rangle \langle \varepsilon \rangle - \langle z \rangle \langle z\varepsilon \rangle + \langle z \rangle^2 \langle \varepsilon \rangle.
\]

(5.75)

Relations (5.70)-(5.75) provide a method in MC simulations for easily sampling the expansion coefficients in the density gradient expansion of both the average energy and electron flux.

In summary, Monte Carlo codes described in this chapter can be viewed as a tool to calculate the bulk and flux transport coefficients and other transport properties under hydrodynamic conditions for static electric and magnetic fields crossed at arbitrary angle (see Chapters 6 and 7) and for time-dependent fields in a crossed field configuration (see Chapter 8) when non-conservative collisions are present. Under non-hydrodynamic conditions when both electric and magnetic fields are present and non-conservative collisions are operative, we can calculate: (i) the spatial profiles of various transport properties and (ii) expansion coefficients in the density gradient expansion of the transport properties including the gradient energy parameter. We are then in a position to assess the accuracy/convergence of the density gradient expansion for the SST average energy and SST average velocity in the far-downstream SST profiles where hydrodynamic conditions generally prevail. This is a program of investigation presented in Chapter 9.
Chapter 6

Benchmark calculation of electron transport in dc electric and magnetic fields crossed at arbitrary angle

6.1 Introduction

The hydrodynamic kinetic theory and associated numerical code developed in previous chapters for the solution of Boltzmann’s equation are tested against the results obtained by a Monte Carlo simulation technique. For that purpose, we have used a serious of model conservative and non-conservative gases including the Reid ramp model (Reid, 1979), the ionization model of Lucas and Saelee (Lucas and Saelee, 1975) and modified attachment model of Ness and Robson (Ness and Robson (1986); Nolan et al. (1997)). The reasons for using Monte Carlo method and model cross sections in benchmark calculations are not always fully appreciated. A Monte Carlo method is based on the first principles with errors which are of a statistical nature only and therefore well understood. On the other hand, through the use of simple forms of cross sections we can isolate and elucidate fundamental physical processes which govern the specific behavior of electron swarm for a given set of simulation conditions. In addition, the analytical form of the cross sections provides no ambiguity and uncertainty generated by the complicated structure of real cross sections. However, it must be emphasized that the theory and numerical codes are applicable for real gases, as discussed in later chapters.

We begin this chapter by investigating the numerical accuracy of our Monte Carlo simulation code using the benchmark Reid ramp model for electron swarms in dc electric and magnetic fields crossed at arbitrary angle. The code has been cross-checked against the results obtained by a multi-term theory for solving the Boltzmann equation (White et al., 1999a). Aside from the Reid ramp model however, there exist no benchmarks in the literature for dc electric and magnetic fields crossed at arbitrary angle when non-conservative collisions are operative. Thus we have employed the ionization model of Lucas and Saelee and modified attachment model of Ness and Robson with the goal of providing benchmarks for future investigations of electron transport.
swarms in dc electric and magnetic fields crossed at arbitrary angles when electron transport is greatly influenced by non-conservative collisions. Transport coefficients and distribution function components for these two model non-conservative gases under the action of a dc electric field have been extensively investigated (Taniguchi et al. (1977); Ness and Robson (1986); Nolan et al. (1997); Raspopović et al. (1999)). In contrast to the magnetic field-free case, there have been limited investigations of electron transport in electric and magnetic fields when non-conservative collisions are operative (Li et al. (2001); Dujko et al. (2005; 2006)). Therefore, in this chapter we present the first systematic treatment of the effect of non-conservative processes on the transport coefficients in dc electric and magnetic field crossed at arbitrary angle.

The second important aspect of the present chapter is to highlight the general features of various electron transport properties in gases under the action of electric and magnetic fields crossed at arbitrary angle when non-conservative collisions are operative. We restrict our discussion and results to the influence of varying the angle between the electric and magnetic field strengths, and consider only a limited number of magnetic field strengths and fix the electric field. However, this is done for a range of model gases with the principal idea to understand the synergism of magnetic fields and non-conservative collisions in electron transport. One point concerning the calculations of transport coefficients is particularly important. In this chapter both the bulk and flux values of transport coefficients are presented. As discussed in Chapter 2 the bulk transport coefficients are experimentally measurable transport quantities and contain both the implicit (i.e., the effects of non-conservative collisions on the distribution function only) and explicit effects of non-conservative collisions. On the other hand, the flux transport coefficients contain the implicit effects only of non-conservative collisions on the transport coefficients. All previous treatments of electron transport in dc electric and magnetic fields crossed at arbitrary angle have neglected the explicit effects of non-conservative processes.

In section 6.2 we examine the Reid ramp inelastic model for dc electric and magnetic fields. In this section the results of benchmarking of our Monte Carlo simulation code are presented. The sections 6.3 and 6.4 concern the influence of ionization and attachment processes on the electron transport coefficients. While the comparisons between the results obtained by a multi-term solution of the Boltzmann equation and Monte Carlo simulation are deferred to the Appendices A and B, the physics associated with electron swarms in electric and magnetic fields at arbitrary angle is considered. Certain trends in the profiles of transport coefficients/properties as a function of the magnetic field strength and angle between the fields are addressed using physical arguments. Finally, in the section 6.5, the two-term approximation and Legendre polynomial expansion are tested against the multi-term solutions of the Boltzmann equation. Similar study has been published recently (White et al., 1999a), but we make a further generalization to consider the influence of non-conservative collisions and both type of transport data, the bulk and flux.
6.2 The Reid ramp model

The Reid ramp model (Reid (1979)) has become the standard test for Monte Carlo simulations (Penetrante et al. (1985); Brennan et al. (1990)) and Boltzmann equation solutions, particularly in the light of known failure of the two-term approximation for this model (Ness (1994); White et al. (1997); Raspopović et al. (1999)). Ness (1994) and Raspopović et al. (1999) extended this model to the orthogonal field configuration. Their results validate both the hydrodynamic theory of Ness (1994) and the numerical accuracy of a Monte Carlo code developed by Raspopović et al. (1999). Further extensions of this model include the work of White et al. (1999a). In their work, the Reid ramp model was extended into the domain of electric and magnetic fields crossed at arbitrary angle. Their results for the electron transport coefficients are compared with those from the present Monte Carlo simulation.

The Reid ramp inelastic model of interaction is given by

\[
\sigma_m(\epsilon) = 6 \text{Å}^2 \quad \text{(elastic cross section)}
\]

\[
\sigma_{inel}(\epsilon) = \begin{cases} 
10(\epsilon - 0.2) \text{ Å}^2, & \epsilon \geq 0.2 \text{ eV} \quad \text{inelastic cross section} \\
0, & \epsilon < 0.2\text{eV}
\end{cases}
\]

\[
m_o = 4 \text{ amu}
\]

\[
T_o = 0 \text{ K}
\]

where \(m_o\) and \(T_o\) represent the mass and temperature of the neutral gas particles while \(\epsilon\) has the units of eV. All electron scattering are assumed to be an isotropic regardless of the collision nature.

The Reid model has been enabled us to test our Monte Carlo code where the electron transport is under the influence of energy dependent collision frequency when electric and magnetic fields are crossed at arbitrary angle. The results of the simulation are presented in Table 1 and compared with those obtained by a multi-term solution of the Boltzmann equation (White et al., 1999a). The results from the simulation are consistent with those predicted by a multi-term solution of the Boltzmann equation over the entire range of \(B/n_0\) and \(\psi\) considered. Agreement is to within 0.5% for the mean energy and drift velocity components and to within 0.6% for diagonal elements of the diffusion tensor. These results support the numerical accuracy and integrity of the present Monte Carlo code. The basic trends in transport coefficients and properties have been recently addressed (White et al., 1999a) and will not be repeated here.
Table 6.1: A comparison of the transport properties for the Reid ramp model as a function of \( \psi \) at \( E/n_o \) of 12 Td and \( B/n_o \) of 50 Hx (a) and 200 Hx (b) using the Monte Carlo code (MC) and multi-term code for solving Boltzmann equation (BE). \( \Delta \) represents the percentage deviation between these two sets of the results.

(a) \( B/n_o = 50 \) Hx

<table>
<thead>
<tr>
<th>( \psi ) (°)</th>
<th>( \epsilon ) (eV)</th>
<th>( W_x ) ( (10^4 \text{ms}^{-1}) )</th>
<th>( W_y ) ( (10^4 \text{ms}^{-1}) )</th>
<th>( W_z ) ( (10^4 \text{ms}^{-1}) )</th>
<th>( n_o D_{xx} ) ( (10^{24} \text{m}^{-1}\text{s}^{-1}) )</th>
<th>( n_o D_{yy} ) ( (10^{24} \text{m}^{-1}\text{s}^{-1}) )</th>
<th>( n_o D_{zz} ) ( (10^{24} \text{m}^{-1}\text{s}^{-1}) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>MC</td>
<td>0.269</td>
<td>—</td>
<td>—</td>
<td>6.839</td>
<td>1.010</td>
<td>1.015</td>
<td>0.569</td>
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<tr>
<td>( \Delta(%) )</td>
<td>0.0</td>
<td>—</td>
<td>—</td>
<td>0.1</td>
<td>0.1</td>
<td>-0.4</td>
<td>0.0</td>
</tr>
<tr>
<td>BE</td>
<td>0.269</td>
<td>—</td>
<td>—</td>
<td>6.838</td>
<td>1.011</td>
<td>1.011</td>
<td>0.569</td>
</tr>
<tr>
<td>( \Delta(%) )</td>
<td>0.0</td>
<td>-0.1</td>
<td>0.4</td>
<td>0.1</td>
<td>-0.2</td>
<td>0.1</td>
<td>0.3</td>
</tr>
<tr>
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<td>-0.957</td>
<td>0.266</td>
<td>6.738</td>
<td>1.025</td>
<td>1.036</td>
<td>0.0</td>
</tr>
<tr>
<td>( \Delta(%) )</td>
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<td>-0.1</td>
<td>0.4</td>
<td>0.1</td>
<td>-0.2</td>
<td>0.1</td>
<td>0.3</td>
</tr>
<tr>
<td>BE</td>
<td>0.267</td>
<td>-0.956</td>
<td>0.265</td>
<td>6.737</td>
<td>0.565</td>
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<td>0.4</td>
<td>0.1</td>
<td>-0.2</td>
<td>0.1</td>
<td>0.3</td>
</tr>
<tr>
<td>MC</td>
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<td>-1.716</td>
<td>0.284</td>
<td>6.521</td>
<td>1.065</td>
<td>1.095</td>
<td>0.558</td>
</tr>
<tr>
<td>( \Delta(%) )</td>
<td>0.0</td>
<td>-0.1</td>
<td>0.4</td>
<td>0.1</td>
<td>-0.2</td>
<td>0.1</td>
<td>0.3</td>
</tr>
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<td>1.065</td>
<td>1.095</td>
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</tr>
<tr>
<td>( \Delta(%) )</td>
<td>0.0</td>
<td>-0.1</td>
<td>0.4</td>
<td>0.1</td>
<td>-0.2</td>
<td>0.1</td>
<td>0.3</td>
</tr>
<tr>
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<td>—</td>
<td>6.401</td>
<td>1.096</td>
<td>1.132</td>
<td>0.557</td>
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<tr>
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<td>0.1</td>
<td>—</td>
<td>0.0</td>
<td>-0.3</td>
<td>0.4</td>
<td>-0.4</td>
</tr>
<tr>
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<td>-2.020</td>
<td>—</td>
<td>6.401</td>
<td>1.093</td>
<td>1.137</td>
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</tr>
</tbody>
</table>

(b) \( B/n_o = 200 \) Hx

<table>
<thead>
<tr>
<th>( \psi ) (°)</th>
<th>( \epsilon ) (eV)</th>
<th>( W_x ) ( (10^4 \text{ms}^{-1}) )</th>
<th>( W_y ) ( (10^4 \text{ms}^{-1}) )</th>
<th>( W_z ) ( (10^4 \text{ms}^{-1}) )</th>
<th>( n_o D_{xx} ) ( (10^{24} \text{m}^{-1}\text{s}^{-1}) )</th>
<th>( n_o D_{yy} ) ( (10^{24} \text{m}^{-1}\text{s}^{-1}) )</th>
<th>( n_o D_{zz} ) ( (10^{24} \text{m}^{-1}\text{s}^{-1}) )</th>
</tr>
</thead>
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<tr>
<td>MC</td>
<td>0.269</td>
<td>—</td>
<td>—</td>
<td>6.839</td>
<td>0.382</td>
<td>0.382</td>
<td>0.569</td>
</tr>
<tr>
<td>( \Delta(%) )</td>
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<td>—</td>
<td>—</td>
<td>-0.1</td>
<td>0.3</td>
<td>0.3</td>
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</tr>
<tr>
<td>BE</td>
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<td>—</td>
<td>—</td>
<td>6.838</td>
<td>0.383</td>
<td>0.383</td>
<td>0.569</td>
</tr>
<tr>
<td>( \Delta(%) )</td>
<td>0.0</td>
<td>-0.1</td>
<td>0.0</td>
<td>-0.1</td>
<td>0.0</td>
<td>-0.2</td>
<td>0.1</td>
</tr>
<tr>
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<td>1.874</td>
<td>6.108</td>
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<td>0.472</td>
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<td>( \Delta(%) )</td>
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<td>-0.1</td>
<td>0.0</td>
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<td>0.0</td>
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<td>0.517</td>
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<tr>
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<td>0.0</td>
<td>-0.1</td>
<td>0.0</td>
<td>-0.2</td>
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<td>4.187</td>
<td>0.329</td>
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</tr>
<tr>
<td>( \Delta(%) )</td>
<td>0.0</td>
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<td>0.0</td>
<td>-0.1</td>
<td>0.0</td>
<td>-0.2</td>
<td>0.1</td>
</tr>
<tr>
<td>BE</td>
<td>0.221</td>
<td>-3.277</td>
<td>2.465</td>
<td>4.186</td>
<td>0.330</td>
<td>0.741</td>
<td>0.392</td>
</tr>
<tr>
<td>( \Delta(%) )</td>
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<td>-0.1</td>
<td>0.0</td>
<td>-0.1</td>
<td>0.0</td>
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<tr>
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<tr>
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<td>—</td>
<td>2.573</td>
<td>0.295</td>
<td>1.129</td>
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6.3 The Ionization model of Lucas and Saelee

For the consideration of ionization processes on the electron transport coefficients and properties we consider the benchmark model of Lucas and Saelee (1975). The details of this model are

\[
\sigma_{\text{el}}(\epsilon) = 4\epsilon^{-1/2} \text{Å}^2 \quad \text{(elastic cross section)}
\]

\[
\sigma_{\text{ex}}(\epsilon) = \begin{cases} 
0.1(1 - F)(\epsilon - 15.6) \text{Å}^2, & \epsilon \geq 15.6 \text{ eV} \\
0, & \epsilon < 15.6 \text{eV}
\end{cases} \quad \text{(inelastic cross section)}
\]

\[
\sigma_I(\epsilon) = \begin{cases} 
0.1F(\epsilon - 15.6) \text{Å}^2, & \epsilon \geq 15.6 \text{ eV} \\
0, & \epsilon < 15.6 \text{eV}
\end{cases} \quad \text{(ionization cross section)}
\]

\[
P(q, \epsilon') = 1, \; m/m_o = 10^{-3}, \; E/n_o = 10 \; \text{Td}, \; T_o = 0 \; \text{K} . \quad (6.2)
\]
In the above cross-section definitions energy is in eV, $T_0$ is the temperature of the neutral gas molecules while $M$ and $m$ denote the molecular and electron masses respectively. The parameter $F$ controls the magnitude of the excitation and ionization cross sections. All scattering events are assumed isotropic and the cross sections listed above are ‘total’ cross sections, that is, integrated over all angles. The ionization partition function $P(q,\epsilon')$ (where $q$ is the fraction of the available energy after ionization given to the ejected electron and $\epsilon'$ is incident energy) is set equal to unity implying that all the fractions $0 \leq q \leq 1$ are equiprobable. As Ness and Robson (1986) pointed out, for sufficiently weak electric fields, the ionization rates are low and hence the electron transport properties are relatively insensitive to the magnitude of the partition function. Therefore, the above assumption is justified. Conversely, for high ionization rates, an accurate knowledge of the partitioning of the available energy between the incident and ejected electrons is required. The sensitivity of the electron transport coefficients to post-ionization energy partitioning has been studied using a Monte Carlo method (Tzeng and Kunhardt, 1986) and multi-term theory for solving the Boltzmann equation (Ness and Nolan, 2000).

The results of benchmark calculations are presented in this section and in the Appendix A. We defer comparisons between the results obtained by a multi-term code for solving Boltzmann equation and Monte Carlo simulations to the Appendix A, and prefer here to develop an appreciation for the physics associated with swarms in electric and magnetic fields at arbitrary angles when the electron swarm is greatly influenced by non-conservative collisions. Calculations have been made for a carefully selected set of input parameters. We consider the reduced electric field of 10 Td, the reduced magnetic field range: 100-1000 Hx and angles between 0 and $\pi/2$ rad. The symmetry properties outlined by (White et al., 1999a) can be used to consider angles greater than $\pi/2$ rad. Calculations are performed for different $F$ parameter. If the model parameter $F$ is set to zero, no ionization occurs. This gas model is then reduced to elastic and excitation cross sections. If the model parameter $F$ is set to 0.5, the cross sections for ionization and excitation have the same magnitude and finally if the model parameter $F$ is set to unity, no excitation occurs. Thus, we use the ionization model of Lucas and Saelee to isolate and separate effects of inelastic and ionization collisions, respectively.

Independent of the parameter $F$, convergence was achieved for $l_{\text{max}} = 2$, indicating inelastic collisions had little effect on the anisotropy of the velocity distribution function. For this model, the two-term approximation generally fails to provide the correct values for the diffusion coefficients. The results from a multi-term theory for solving Boltzmann equation are consistent with those predicted by a Monte Carlo simulation code over the entire range of $B/n_0$ and $\psi$ considered in this work (see Appendix A). In all cases, agreement is very good within the statistical uncertainty of Monte Carlo results.

Following the previous works of Dujko et al. (2005; 2006), we often find it convenient to refer to the charged-particle trajectories to explain certain trends in the profiles of the transport coefficients. In the absence of collisions, electrons gyrate about the magnetic field lines at a frequency $\Omega = eB/m$ and with a Larmor radius $r = mc_T/eB$, where $c_T$ is the tangential speed of the orbit. When collisions become important, it is convenient to break up the electron
transport into three regions depending upon the relative strength of the magnetic field and the collisional processes. First, there is a collision-dominated regime ($\Omega \ll k_{tot}$, where $k_{tot}$ is the total collision rate) where electrons may complete only a part of their orbits between successive collisions. Second, there is an intermediate regime ($\Omega \approx k_{tot}$) where the motion of electrons is very complicated. Finally, there is a magnetic field-controlled regime ($\Omega \gg k_{tot}$) where electrons on average complete many circular orbits per collision. Classification of these regimes can be made through the comparison between the total collision rate and cyclotron frequency (Dujko et al. (2005; 2006)).

6.3.1 Mean energy and ionization rate

In figure 6.1 (a) we show the variation of the mean energy $\varepsilon$ with $\psi$ for $B/n_0$ of 100, 200 and 1000 Hx at $E/n_0$ of 10 Td. The mean energy monotonically decreases with $\psi$ and/or $B/n_0$ for all $F$. This is the well-known phenomenon of ‘magnetic cooling’ and it results from an inability of the electric field to efficiently pump the energy into the system (Ness, 1994) because the electrons change the direction of motion due to the magnetic field. This phenomenon is enhanced as the component of the magnetic field perpendicular to the electric field is increased. It is interesting to note that this phenomenon is independent of the gas considered and has been observed previously for all model (Ness (1994); White et al. (1999a) and real (White et al. (1999d); White et al. (2005); Dujko et al. (2005; 2006)) gases. Only recently it has been shown that for a very narrow range of conditions the mean energy may begin to rise with the magnetic field (Ness and Makabe, 2000). In particular, for parallel fields ($\psi = 0$), on average the electrons are traveling in the direction of the electric and magnetic field and hence the magnetic field has no explicit effect. Consequently the mean energy is independent of $B/n_0$.

In figure 6.1 (a), we observe that mean energy decreases when increasing $F$ for fixed $B/n_0$ and $\psi$ in the collision-dominated regime. After an ionization process, the remaining energy is always shared between two electrons while in case of inelastic collision, the remaining energy is held by only one electron. As a consequence, the mean energy after ionization is lower than that after inelastic collision, a phenomenon usually called energy dilution due to ionization (Robson and Ness, 1988). The phenomenon of ionization cooling of the swarm is well-known in dc electric fields and is shown in figure 6.1 (a) to carry over directly to crossed dc electric and magnetic fields but only in the collision-dominated regime. As the angle between the fields increases for $B/n_0$ of 1000 Hx (magnetic field-controlled regime) this phenomenon is significantly reduced. The application of a magnetic field leads to the Maxwellization of high-energy electrons and as a result the influence of both the excitation and ionization processes is significantly reduced. The reduction of the ionization rate for an increasing $B/n_0$ and/or $\psi$ is clearly evident from figure 6.1 (b).
6.3.2 Drift speed, drift velocity components and gradient energy vector components

For the ionization model of Lucas and Saelee, the drift speed is a one-to-one function of the mean energy, and hence the drift speed shows the same trends as the mean energy, as shown in figure 6.2 (a). For this model, the implicit effect of ionization on the drift velocity is weak, and the flux components for \( F = 0.5 \) and \( F = 1 \) are essentially equal to the \( F = 0 \) profile. Therefore, in figure 6.2 (a) the flux component for \( F = 0 \) is shown only. As \( B/n_0 \) and/or \( \psi \) increase, both the bulk and flux values of the drift speed monotonically decrease. This is not a general rule; the exceptions are the gases which give rise to negative differential conductivity. Typical examples include methane (Bzenić et al. (1999); White et al. (1999d); Ness and Nolan (2000)) and carbon-tetrafluoride (Dujko et al. (2005; 2006)).

The drift velocity components \( W_x \) and \( W_y \) satisfy the following symmetry properties (White et al., 1999a): \( W_x = W_y = 0 \) for \( \psi = 0 \) and \( W_y = 0 \) for \( \psi = 90^\circ \). In figure 6.2 (b) we show the bulk and flux values of the drift velocity component along the \( z \)-direction while in figures 6.3 (a) and (b) the drift velocity components along the \( x \) and \( y \) directions are shown. For clarity, in figure 6.3 (a) we show only the flux values of \( W_x \) since there are no differences between flux and bulk components for this drift velocity component for all \( \psi \) considered. Two interesting properties are clearly evident from these profiles: (i) for an increasing \( \psi \), \( W_x \) monotonically increases, \( W_y \) has a maximal property and \( W_z \) monotonically decreases; (ii) for a fixed angle between the fields \( \psi \), the magnitudes of \( W_x \), \( W_y \) and \( W_z \) display respectively the maximal property, monotonically increase and monotonically decrease as \( B/n_0 \) is increased. These properties are quite general.
and have been previously observed for model (White et al., 1999a) and real gases (White et al. (2005); Dujko et al. (2006)). It is interesting to note that the flux $W_y$-profiles follow the sin$2\psi$-dependence while the corresponding profiles of the bulk components are slightly shifted to the right indicating the complex variation of the averaged energy along the swarm in $y$-direction. As expected, the deviations between the flux and bulk components of $W_z$ are diminished as the angle $\psi$ is increased for all $B/n_0$ considered. In particular, in the magnetic field-controlled regime ($B/n_0$ of 1000 Hx and $\psi > 70^\circ$) there are no differences between the bulk and flux components of both $W_y$ and $W_z$.

Let us consider now the origin of differences between the bulk and flux components of the drift velocity components. To study in detail the effect of non-conservative collisions on electron transport, we need to consider the spatial profile of the average energy through the swarm. As pointed out by Li et al. (2001), the gradient energy vector plays a key role in physical understanding of the effects of non-conservative collisions on electron transport coefficients. For an arbitrary field configuration studied here, the gradient energy vector $\gamma$ satisfies the following symmetry conditions: $\gamma_x = \gamma_y = 0$ for $\psi = 0$ and $\gamma_y = 0$ for $\psi = 90^\circ$. These symmetry properties are independent of the gas considered. In figures 6.4 (a) and (b) we show the $y$ and $z$ components of this transport property as a function of $B/n_0$ and $\psi$. The $x$-component is shown in figure 6.5. As can be observed, $\gamma_y$ displays a maximal property for all $B/n_0$ considered here with respect to $\psi$ while $\gamma_z$ monotonically increases for $B/n_0$ of 100 and 200 Hx and displays a maximal property for $B/n_0$ of 1000 Hx. In the collision-dominated regime and for the angles up to $\psi = 60^\circ$, $\gamma_y$ is an increasing function of $B/n_0$ and decreasing function of the parameter $F$. However, as $\psi$ is further increased, there are no differences between the $\gamma_y$ profiles for all
Figure 6.3: Variation of the $x$- (a) and $y$- (b) drift velocity components as a function of $B/n_0$ and $\psi$ for the ionization model of Lucas and Saelee for the same conditions as those in Fig. 6.2. $F$ considered. Similar behavior can be observed in the profiles of $\gamma_z$ but only for $B/n_0$ of 1000 Hx. Another striking feature is the fact that both $\gamma_y$ and $\gamma_z$ are negative (or zero) for all $\psi$, indicating the average energy increases through the swarm in these directions in the direction that the swarm is drifting.

Figure 6.4: Variation of the $y$- and $z$-components of the gradient energy vector as a function of $B/n_0$ and $\psi$ for the ionization model of Lucas and Saelee for the same conditions as those in Fig. 6.1.

In figure 6.5 we show the $x$-component of the gradient energy vector $\gamma_x$, as a function of $B/n_0$ and $\psi$. We observe that in contrast to $y$- and $z$-direction, there is a very little spatial variation in the average energy along the $x$-axis ($E \times B$ direction). Further and in contrast to
\( \gamma_y \) and \( \gamma_z \), the spatial variation in the average energy in the \( \mathbf{E} \times \mathbf{B} \)-direction is in the opposite direction to the drift in that direction. This unexpected behavior of \( \gamma_x \) supports the previous works of Li et al. (2001) and Dujko et al. (2005; 2006).

![Figure 6.5: Variation of the \( x \)-component of the gradient energy vector as a function of \( B/n_0 \) and \( \psi \) for the ionization model of Lucas and Saelee for the same conditions as those in Fig. 6.1.](image)

Generally speaking, the distinction between flux and bulk components of the drift velocity vector elements is a consequence of spatially dependent non-conservative collisions resulting from a spatial variation of average electron energies within the swarm (Ness and Robson, 1986). If the ionization rate is an increasing function of electron energy, electrons are preferentially created in regions of higher energy resulting in a shift in the centre of mass position as well as a modification of the spread about the centre of mass. For the ionization model of Lucas and Saelee and field configuration studied here, the electrons are preferentially created at the front of the swarm in the \( z \)-direction and hence the magnitude of the bulk drift component in this direction is greater than the equivalent flux component. The same physical picture applies for drift in the \( y \)-direction.

When we consider the drift velocity component along the \( \mathbf{E} \times \mathbf{B} \) direction, the picture is not as simple. The drift velocity component along the \( \mathbf{E} \times \mathbf{B} \) direction \( W_x \), appears in general to be less sensitive to the effects of ionization processes. This weak sensitivity of \( W_x \) to the ionization processes is indicative of an essentially symmetric spatial profile (with a slight bias) of average energy about the centre of mass of the swarm in the \( \mathbf{E} \times \mathbf{B} \) direction. Consequently, the essentially symmetric production of electrons about the centre of mass by ionization process do not have a major impact on the position of the centroid, and the small differences between bulk and flux components in this direction then follow. These small differences are due to the slight non-symmetrical bias in the spatial variation of the average energy in that direction. Further and in contrast to both the \( y \)- and \( z \)-directions, where the average energy increases in the direction of the drift in these directions (independent of the electric field strength), in the \( x \) direction the spatial variation is dependent on the magnitude of the electric field. Recent
studies on non-conservative electron transport in the presence of electric and magnetic fields for CF$_4$ using a Monte Carlo simulation technique (Dujko et al., 2006) and for argon using a multi-term Boltzmann analysis (White et al., 2002) have revealed that for low $E/n_0$ the average energy decreases in the direction of the drift. Hence, for CF$_4$ at fields where attachment is the dominant non-conservative process, the bulk is greater than the flux while for argon due to the absence of attachment the opposite situation holds: the flux is greater than the bulk. In case of CF$_4$, as $E/n_0$ increases and the ionization becomes dominant non-conservative process, there is a transition process where the flux is greater than the bulk to the normal situation where the average energy increases in the direction of the drift and consequently, the bulk is greater than the flux. It is important to note that this transition process can be controlled by the angle between the fields. In any case, the synergism of large energy losses in inelastic collisions and strong influence of the ionization processes restore the regime where the bulk is greater than the flux which is consistent with the other directions.

6.3.3 Diagonal elements of the diffusion tensor

The variation of the flux diagonal elements of the diffusion tensor along the $x$- and $z$-directions, $n_0D_{xx}$ and $n_0D_{zz}$, with $B/n_0$ and $\psi$ for all $F$ considered is shown in figures 6.6 (a) and (b). In figure 6.7 we display the variation of the flux components of $D_{yy}$. In contrast to the drift velocity components, the implicit effects of the ionization processes on the diagonal elements of the diffusion tensor are quite strong and hence we observe different profiles for different ionization degrees $F$. Due to the complexity and interplay of various factors which influence the diffusion tensor it is hard to fully understand and elucidate even the basic trends in the profiles of the diffusion tensor components. These factors include: (a) the thermal anisotropy effect resulting from the different random electron motions in different directions, (b) the magnetic anisotropy effect which acts to inhibit diffusion in the plane perpendicular to the magnetic field and (c) the electric anisotropy effect arising from a spatial variation of the average energy and local average velocities throughout the swarm which act so as to either inhibit or enhance diffusion. In addition to this triple anisotropy effect, the effects of collisions, energy dependent total collision frequency and further couplings of these factors can further complicate the physical content of this issue. A convenient way to isolate and elucidate the phenomena associated only with the field effects is using a simple analytical form of cross sections in the calculations (White et al., 1999a). For the ionization model of Lucas and Saelee the electric anisotropy is almost absent by virtue of the almost energy independent collision frequency. In addition, the thermal anisotropy is also significantly reduced indicating the fact that this model enables us to study the synergism of the anisotropy introduced by explicit orbital effects (the magnetic field anisotropy effect) and the effects of ionization processes. The previous study of White et al. (1999a) unearthed some generic features of the diffusion tensor components which are again observed for the ionization model of Lucas and Saelee. We highlight these features and focus on a unique aspect for the ionization model of Lucas and Saelee and the explicit effects of non-conservative collisions on the diagonal diffusion tensor components.
Figure 6.6: Variation of the flux components of $n_0 D_{xx}$ (a) and $n_0 D_{zz}$ (b) as a function of $B/n_0$ and $\psi$ for the ionization model of Lucas and Saelee. The solid, dashed and dotted lines (black: 100 Hx; red: 500 Hx; blue: 1000 Hx) represent $n_0 D_{xx}$ and $n_0 D_{zz}$ for $F = 0$, $F = 0.5$ and $F = 1$, respectively.

From figures 6.6 (a) and (b) and figure 6.7 we observe that for a fixed $B/n_0$, $n_0 D_{xx}$ and $n_0 D_{zz}$ are monotonically decreasing functions of $\psi$, while $n_0 D_{yy}$ displays a non-symmetrical maximal property with $\psi$. For a given $\psi$, we observe that both $n_0 D_{xx}$ and $n_0 D_{yy}$ are monotonically decreasing functions of $B/n_0$, as is $n_0 D_{zz}$ provided $\psi \neq 0$. For parallel fields ($\psi = 0^\circ$), the diffusion is isotropic in the plane perpendicular to $B$, i.e. $n_0 D_{xx} = n_0 D_{yy}$ which can be expected from the symmetry properties (White et al., 1999a). In addition, for parallel field configuration $n_0 D_{zz}$ is independent of $B/n_0$ while $n_0 D_{xx}$ and $n_0 D_{yy}$ are monotonically decreasing functions of $B/n_0$. On the other hand, in a crossed field configuration ($\psi = 90^\circ$), the diffusion is isotropic in the plane perpendicular to $B$. These are typical examples of the magnetic field anisotropy of the diffusion tensor.

The variation of the diagonal diffusion tensor elements with $B/n_0$ and $\psi$ for the ionization model of Lucas and Saelee is dominantly induced by the thermal and magnetic field anisotropy effects. The thermal contribution is a decreasing function of both $B/n_0$ and $\psi$ (see the components of the temperature tensor displayed below). On the other hand, the magnetic field acts to inhibit diffusion in a plane perpendicular to itself. This effect is further strengthened as the magnetic field is increased due to the fact that the electron complete a greater fraction and number of orbits before undergoing a collision. Note that as $B/n_0$ increases, both $D_{xx}$ and $D_{zz}$ may vary over several orders of magnitude. While the inhibiting explicit orbital effect is strengthened with $\psi$ for $D_{zz}$, the same effect is much less pronounced for $D_{xx}$. Consequently, $D_{zz}$ monotonically and markedly decreases with $\psi$ while $D_{xx}$ is less sensitive to $\psi$.

The diffusion coefficient $n_0 D_{yy}$, shown in figure 6.7 stands in contrast to both $D_{xx}$ and $D_{zz}$. The variation in $n_0 D_{yy}$ with $B/n_0$ is relatively small when compared to that for diffusion.
Figure 6.7: Variation of the flux components of $n_0 D_{yy}$ as a function of $B/n_0$ and $\psi$ for the ionization model of Lucas and Saelee for the same conditions as those in Fig. 6.6.

perpendicular to the magnetic field. The reason for this is that there is no explicit orbital effect on diffusion parallel to the magnetic field, and diffusion is purely thermal. For non-orthogonal field configuration, the variations of thermal and orbital effects with $\psi$ tend to oppose each other, and hence $n_0 D_{yy}$ shows the maximal property with $\psi$.

In what follows the influence of ionization on the diagonal elements of the diffusion tensor is analyzed by considering the difference between the bulk and flux values of a given transport property. In figures 6.8 (a) and (b) and figure 6.9 we show the percentage difference $\Delta$ between the bulk and flux components of the diagonal elements of the diffusion tensor as a function of $B/n_0$ and $\psi$ where

$$\Delta = \frac{|\text{bulk}| - |\text{flux}|}{|\text{bulk}|} \times 100\%.$$  \hspace{1cm} (6.3)

For illustrative purpose, we chose $B/n_0$ of 100, 200 and 500 Hx. From figures 6.8 (a) and (b) and figure 6.9 it is seen that differences between the bulk coefficients and their flux components can be greater than 25%. For $n_0 D_{yy}$ and $n_0 D_{zz}$ the bulks are always greater than the corresponding flux components. This indicates that the increase in electron numbers due to ionization enhances diffusion in both $y$- and $z$- directions. On the other hand, from Figure 8.9 it is seen that for both $F = 0.5$ and $F = 1$ subject to a $B/n_0$ of 500 Hx, the flux can be greater than the corresponding bulk components. Similar but not identical trends have been recently observed for the model and real gases for orthogonal field configuration.

In contrast to the drift velocity components, the explicit effects of ionization on the diagonal elements of the diffusion tensor are dependent on both the first order ($\gamma$) and the second order ($\zeta$) variations of the average energy through the swarm (see eq. (2.124)). These quantities have been previously defined through a density gradient expansion of the average energy (see Eq. 2.124). The spatial variation of the average energy profile through the swarm is determined by.
Figure 6.8: The percentage difference between the bulk and flux values of $n_0 D_{yy}$ and $n_0 D_{zz}$ as a function of $\psi$ for $B/n_0$ of 100, 200 and 500 Hx.

Figure 6.9: The percentage difference between the bulk and flux values of $n_0 D_{xx}$ as a function of $\psi$ for $B/n_0$ of 100, 200 and 500 Hx.

$\gamma$ and/or $\zeta$ and hence there exist preferential creation of the electrons in certain directions if the ionization rate is energy dependent. This is the reason for the explicit modification of diffusion. The application of a magnetic field at arbitrary angle with respect to the electric field further modifies the spatial variation of the average energy profile and in general both $\gamma$ and $\zeta$ are complex functions of $B/n_0$ and $\psi$. We may observe that the differences between the bulk and flux components for all diagonal diffusion elements are relatively insensitive with respect to the angle between the fields for low $B/n_0$. This is due to the small variations of the average energy along the swarm. However, if $B/n_0$ is increased, then the sensitivity of $\Delta$ is greatly increased.
It is interesting to note that various diagonal elements of the diffusion tensor show different sensitivity to $\gamma$ and/or $\zeta$. As an illustrative example, the difference between the bulk and flux components for $n_0 D_{yy}$ and $n_0 D_{zz}$ can be associated with the first order variation of the average energy ($\gamma$). We can see that the peak positions of $n_0 \gamma_y$ and $n_0 \gamma_z$ approximately correspond to peak positions of $\Delta(n_0 D_{xx})$ and $\Delta(n_0 D_{zz})$, respectively, reflecting the high sensitivity of these diffusion coefficients to the first order variation of the average energy through the swarm. On the other hand, $n_0 D_{xx}$ stands in contrast to both $n_0 D_{yy}$ and $n_0 D_{zz}$. As we have said above, there is a very little spatial variation in the average energy along the $x$-axis. To understand the effect of ionization on $n_0 D_{xx}$, a comprehensive investigation of spatially dependent average energy and velocity is inevitable. In particular, the variation of the diffusive energy tensor $\zeta$ with both $B/n_0$ and $\psi$ must be studied. This is beyond the scope of this thesis and we defer this to a future study.

### 6.3.4 Off-diagonal elements of the diffusion tensor

In figure 6.10 we show the off-diagonal elements of the diffusion tensor as a function of $B/n_0$ and $\psi$. The implicit effects of the ionization processes on the off-diagonal elements of the diffusion tensor are quite strong and hence different profiles for different ionization degrees $F$ are clearly evident. The profiles are a monotonically decreasing function of the parameter $F$. In addition, we note for all $B/n_0$ and $\psi$ that

$$D_{xy} \approx -D_{yx}, \quad D_{xz} \approx -D_{yz}, \quad D_{yz} \approx D_{zy}.$$ 

Note that only for the Maxwell model where the collision frequency is independent of energy, the relation operator $\approx$ should be replaced by the operator $=$ (White et al., 1999a). If inelastic collisions start to play significant role, then the symmetry properties for the off-diagonal elements of the diffusion tensor outlined by White et al. (1999a) do not hold any more.

For the ionization model of Lucas and Saelee the off-diagonal elements of the diffusion tensor arises from the interaction of the gradient-induced fluxes with the magnetic field. Consider for example orthogonal field configuration. A density gradient in the $x$ direction will cause a diffusive flux in the $x$ direction. This flux could then interact with the magnetic field to again produce a flux in the $z$ direction. Therefore, a gradient in the $x$ direction can cause a flux in the $z$ direction (described by $D_{xz}$) and a flux in the $x$ direction (described by $D_{xx}$), but not one in the $y$ direction. Hence for the orthogonal field configuration, symmetry properties follow and the coefficient $D_{yz}$ is zero. These effects may be generally categorized as Hall currents, familiar in the plasma physics literature (White et al., 1999a). In particular, it is well documented that for the orthogonal field configuration the Hall diffusion coefficient can have magnitudes of equivalent order to those of diagonal elements (Ness (1994); White et al. (1997; 1999a); Raspopović et al. (1999)). In this thesis we observe the similar trends which is a clear sign that the off-diagonal elements of the diffusion tensor must be considered in fluid modeling of plasma discharges.

There is another interesting aspect associated with the off-diagonal elements of the diffusion tensor: non-conservative collisions do not have explicit effects on individual elements. As an
Figure 6.10: Variation of the off-diagonal elements of the diffusion tensor as a function of $B/n_0$ and $\psi$ for the ionization model of Lucas and Saelee for the same conditions as those in Fig. 6.6.

Illustrative example, the off-diagonal elements of the diffusion tensor for a crossed field configuration are usually reported as the sum $D_h = D_{xz} + D_{zx}$, which appears in the continuity equation. This is the well-known Hall diffusion coefficient and for this transport property the reactive corrections to the bulk component can be found. However, for the individual elements, $D_{xz}$ and $D_{zx}$ the reactive corrections cannot be found. As discussed in Chapter 2, the expressions for the off-diagonal elements of the diffusion tensor cannot be directly obtained from the diffusion equation but rather must be obtained from the flux-gradient relation. This is a result of the parity and symmetry properties imposed on the distribution function, independently of
the configuration of electric and magnetic fields.

In figure 6.11 (a) we display the variation of the flux Hall diffusion coefficient as a function of $B/n_0$ for all $F$ considered. For the weak values of $B/n_0$, we observe different profiles for different ionization degrees $F$ indicating a strong implicit effects of the ionization processes on this transport property. For an increasing $B/n_0$, however, these effects are significantly reduced. As can be observed, the Hall diffusion coefficient exhibits a non-symmetrical profile, peaks at $B/n_0$ of around 80 Hx and then decreases markedly. In fact, the Hall diffusion coefficient may vary over several order of magnitude with $B/n_0$. Finally, for the sake of completeness, the bulk and flux Hall diffusion coefficients for $F = 1$ are shown in figure 6.11 (b). The effects of the ionization processes are obvious through the difference between the flux and bulk data.

### 6.3.5 The diagonal elements of the temperature tensor

In this section we consider the elements of the temperature tensor. The temperature tensor is symmetric and in general full. The components of this transport property satisfy the symmetry properties outlined by White et al. (1999a).

![Figure 6.12: Variation of the diagonal elements of the temperature tensor as a function of $B/n_0$ and $\psi$ for the ionization model of Lucas and Saelee for the same conditions as those in Fig. 6.1.](image)

In figure 6.12 we observe that the diagonal elements of the temperature tensor for the ionization model of Lucas and Saelee generally decrease with $B/n_0$ and $\psi$. This trend is enhanced as the component of the magnetic field perpendicular to the electric field is increased. As can be observed, the profiles of the diagonal elements of the temperature tensor resemble to those of the mean energy which is a general property, independent of the gas. All diagonal elements of the temperature tensor are decreasing functions of the parameter $F$ which is another analogy with the mean energy. Thermal anisotropy for the ionization model of Lucas and Saelee is weak, indicating almost isotropy of the distribution function in velocity space. This is another confirmation that two-term approximation is generally acceptable for solving the Boltzmann equation for this model gas (except for the calculation of the diffusion coefficients). Significant
inelastic processes are in general required to generate significant anisotropy in the temperature tensor.

6.4 The modified attachment model of Ness and Robson

For the consideration of electron attachment processes on the electron transport coefficients and properties we consider the modified attachment benchmark model of Ness and Robson (1986). This model is given by:

\[ \sigma_{el}(\epsilon) = 4\epsilon^{-1/2} \text{Å}^2 \]  
\[ \sigma_{ex}(\epsilon) = \begin{cases} 
0.1(\epsilon - 15.6) \text{Å}^2, & \epsilon \geq 15.6 \text{ eV} \\
0, & \epsilon < 15.6 \text{ eV} 
\end{cases} \]  
\[ \sigma_a(\epsilon) = ae^p \]  
\[ m/m_o = 10^{-3} \]  
\[ E/n_o = 10 \text{ Td} \]  
\[ T_o = 0 \text{ K}. \]  

The parameter \( a \) determines the magnitude while the parameter \( p \) determines the energy dependence of the attachment cross section. This thesis considers \( p = 0.5, -0.5, -1 \). That is, case studies of attachment cross sections directly proportional to the electron velocity, inversely proportional to the electron velocity and inversely proportional to the electron energy. When employing the attachment cross section directly proportional to the electron velocity, we consider the following attachment amplitudes: \( a = 0.3, 0.5 \). In contrast to attachment model studied by Ness (1985) and Ness and Robson (1986), the attachment model considered in this thesis incorporates the inelastic collisions. Since there are no published results for this particular model, we compare results for transport coefficients obtained by a multi-term Boltzmann code with those obtained a Monte Carlo simulation code. We apply the same strategy in this section as in previous one: the results of our benchmark calculations are presented in this section and in the Appendix B. To illustrate the wide spectrum of phenomena associated with the synergism of magnetic field and attachment processes in electron transport, the electron transport coefficients as a function of both \( B/n_0 \) and \( \psi \) will be considered in the succeeding representation.

Since inelastic collisions play an important role in this model, independent of the power \( p \) and attachment amplitude \( a \), convergence was achieved in for \( l_{\text{max}} = 2 \). As pointed out by Ness (1985) and Ness and Robson (1986), attachment has little effect on the isotropy of the velocity distribution function. The anisotropy of the velocity distribution function is induced by an active role of inelastic collisions and hence the two-term approximation generally fails for this model. It has been observed that diffusion coefficients are the most sensitive to the variation of the \( l \)-index. The deviations between diffusion coefficients between the two- and three-term calculations could be up to 20%.

Another important aspect for this model is the case \( p = -0.5 \), where the attachment collision frequency is independent of energy. For such a power law, all bulk transport coefficients (aside
from the attachment rate) were found to be independent of the attachment amplitude and equal to the corresponding flux values. This supports the numerical integrity of the present code in the presence of attachment collisions. For clarity, the electron transport properties for this particular case within modified attachment model of Ness and Robson will not be shown and explicitly labeled.

6.4.1 Mean energy and attachment rate

Figures 6.13 (a) and (b) show the variation of the mean energy $\varepsilon$ and the attachment rate $k_{\text{att}}$, respectively, with $\psi$ for $B/n_0$ of 100, 200 and 1000 Hx at $E/n_0$ of 10 Td. The mean energy monotonically decreases with $B/n_0$ and $\psi$ for both the conservative and non-conservative cases. The attachment rate decreases with $B/n_0$ and/or $\psi$ when the attachment cross section is directly proportional to the electron velocity. On the other hand, when the attachment cross section is inversely proportional to the electron energy, the attachment rate increases with $B/n_0$ and/or $\psi$. When the attachment cross section is directly proportional to the electron speed the high energy electrons are preferentially lost due to the attachment which lowers the swarm mean energy. Increasing the attachment amplitude from $a = 0.3$ to $a = 0.5$ further increases the cooling of the swarm. This process is known as attachment cooling, a phenomenon which was explained in a great detail by Ness and Robson (1986) using the simple analytical form of the cross sections. In addition to model gases, this phenomenon has been observed for a wide range of real electronegative gases where the electron attachment plays important role in electron kinetics. As can be observed from figure 6.13 (b) the attachment cooling directly carries over to a crossed field configuration but with some modifications. When the collisions dominate the electron transport this phenomenon is clearly evident. However, as the electron transport enters the magnetic field-controlled regime the effects of attachment are significantly reduced. In the limit of the perpendicular fields and the highest $B/n_0$ of 1000 Hx, the effects of attachment are essentially removed. Under these extreme conditions, the attachment rate sharply drops-off and the cooling effects induced by the perpendicular component of the magnetic field prevail. Hence the synergism of the magnetic field and attachment cooling mechanism can be controlled through the variation of $B/n_0$ and/or $\psi$. On the other hand, when the electron attachment is inversely proportional to the electron energy, the opposite situation occurs where low-energy electrons are preferentially lost. This is known as the attachment heating, a phenomenon which was introduced in transport theory by Ness and Robson (1986). While the attachment cooling mechanism is significantly reduced in the limit of high $B/n_0$ and $\psi$, the attachment heating mechanism is much less affected by the variation of $B/n_0$ and/or $\psi$. The reason for this is the competition between two essentially opposite processes: the magnetic cooling and the attachment heating. While the magnetic field always acts to decrease the mean energy, the electron attachment give rise to the mean energy. Even in the limit of the highest $B/n_0$ of 1000 Hx and orthogonal field configuration, a remarkable difference in the mean energy between the conservative and non-conservative (attachment heating) models is clearly evident.
Figure 6.13: Variation of the mean energy and attachment rate as a function of $B/n_0$ and $\psi$ for the modified attachment model of Ness and Robson. Black, red, green and blue lines (solid lines: 100 Hx; dashed lines: 200 Hx; dotted lines: 1000 Hx) represent the mean energies for conservative (no attachment) case, non-conservative cases when the attachment cross section is directly proportional to the electron velocity with the attachment amplitudes $a = 0.3$ and $a = 0.5$, and non-conservative case when the electron attachment is inversely proportional to the electron energy, respectively.

6.4.2 Drift speed, drift velocity components and gradient energy vector components

In figures 6.14 (a) and (b) we show the variation of the drift speed and $z$-component of the drift velocity with $\psi$ for $B/n_0$ of 100, 200 and 1000 Hx at $E/n_0$ of 10 Td. The implicit effects of the electron attachment on the drift velocity is weak and hence there are no differences between the flux components associated with different models. The curves show expected decrease in their magnitudes with $B/n_0$ and/or $\psi$. The drift speed is one-to-one function of the mean energy and hence the drift speed shows the same trends as the mean energy. When the attachment is directly proportional to the electron velocity (the so-called attachment cooling model), the more faster electrons tend to be at the front of the traveling swarm and these electrons are preferentially attached. It follows that the attachment will tend to move the center of mass of the swarm in the direction opposite to the drift. Thus the bulk drift speed decreases with respect to the flux component. In addition, the bulk drift speed decreases with the increasing $a$. However, only when the attachment cross section is comparable with the elastic cross section we observe differences between the bulk and flux components. In the limit of the highest $B/n_0$ and $\psi$ considered in this work, these differences are entirely removed. This indicates that for this particular model, the magnetic field acts to suppress the effects of the electron attachment. The same physical picture applies for $W_z$.

When the attachment is inversely proportional to the electron energy (the so-called at-
Figure 6.14: Variation of the drift speed and $W_z$ as a function of $B/n_0$ and $\psi$ for the modified attachment model of Ness and Robson. Black lines represent the flux values while red, green and blue lines represent the bulk values when the attachment cross section is directly proportional to the electron velocity with the attachment amplitudes $a = 0.3$ and $a = 0.5$, and when the electron attachment is inversely proportional to the electron energy, respectively (solid lines: 100 Hx; dashed lines: 200 Hx; dotted lines: 1000 Hx).

tachment heating model), as expected, the opposite physical situation occurs. Now the slower electrons at the back of the swarm are preferentially attached, and so the attachment tend to move the center of mass in the drift direction. Thus the bulk drift speed is greater than the corresponding flux component. Concerning the explicit influence of the electron attachment on the drift speed, it is observed from figure 6.14 (a) that even for the highest $B/n_0$ and $\psi$ when the effects of the magnetic field are the strongest, the effects of the electron attachment are still operative and strongly affect the drift speed.

In figures 6.15 (a) and (b) we show the bulk and flux components of $W_x$ and $W_y$ as a function of $B/n_0$ and $\psi$. While the flux $W_x$-profiles monotonically increase with increasing $\psi$ for all $B/n_0$ considered, the flux $W_y$-profiles follow the $\sin 2\psi$-dependence. There are no differences between the bulk and flux components associated with $W_x$ and hence the flux components are only presented. This is indicative of a small spatial variation in the average energy along the swarm in the $E \times B$ direction. Conversely, the large differences between the bulk and flux components associated with $W_y$ are observed from figure 6.15 (b). For the attachment cooling model the bulk components are less than the flux components. This difference is further increased when increasing the amplitude of the attachment cross section $a$. On the other hand, for the attachment heating model the bulk components are greater than the flux. Interestingly, the difference between the bulk and flux components is more pronounced for higher $B/n_0$ and $\psi$. Starting from a few percents, the difference between the bulk and flux component is increased up to 40% for $B/n_0$ of 1000 Hx and $\psi$ of 70°. This is an evidence how the magnetic field can
favor in a dramatic manner the influence of non-conservative collisions on the electron transport property.

To clarify the differences between the bulk and flux components of the drift velocity components, in figures 6.16 (a) and (b) we display the variation of the y- and z-components of the gradient energy vector as a function of $B/n_0$ and $\psi$. It can be observed that $\gamma_y$ exhibits a non-symmetrical profile with $\psi$ and $B/n_0$ for all attachment models considered. Consequently, the bulk components of $W_y$ are shifted to the right. One the most striking property observed in the profile of $\gamma_z$ is the crossing point between curves representing two different attachment amplitudes. For $B/n_0$ of 200 Hx the crossing point occurs at around $\psi = 55^\circ$ while for $B/n_0$ of 1000 Hx the crossing point occurs at around $\psi = 45^\circ$. However there are no imprints of this phenomenon on the differences between the flux and bulk components. As already remarked, there is a little spatial variation in the average energy along the x-direction with increasing $B/n_0$ and $\psi$. The deviations between the bulk and flux components of $W_x$ are less than 1% for all attachment models.

### 6.4.3 Diagonal elements of the diffusion tensor

In this section the behavior of the diagonal elements of the diffusion tensor is investigated. The variation of the flux diagonal elements of the diffusion tensor with $B/n_0$ and $\psi$ is shown in figures 6.17 (a) and (b) and figure 6.18. In contrast to the drift velocity components, the implicit effects of the attachment upon the diagonal elements of the diffusion tensor are quite strong and different profiles associated with different attachment models can be observed.

For both the attachment cooling and attachment heating models, the magnetic field acts to decrease both $D_{xx}$ and $D_{zz}$. As can be observed, for fixed $\psi$ these two diffusion coefficients
may vary over several orders of magnitude. While $D_{xx}$ has limited sensitivity with respect to $\psi$, the important property of both $D_{yy}$ and $D_{zz}$ is high sensitivity to $\psi$. For the attachment cooling model, it can be observed that the diagonal diffusion coefficients tend to decrease as the attachment amplitude $a$ increases. In other words, the attachment cooling effect decreases the diffusion as it does drift. This is true when the collisions dominate the electron transport while in the limit of high $B/n_0$ and $\psi$ the effects of attachment are significantly reduced. On the other hand, the attachment heating increases diagonal elements of the diffusion tensor as it does drift. In contrast to the attachment cooling model, in the magnetic field-controlled regime
Figure 6.18: Variation of the flux component of $n_0 D_{yy}$ as a function of $B/n_0$ and $\psi$ for the modified attachment model of Ness and Robson for the same conditions as in Fig. 6.13.

The difference in diffusion coefficients between the conservative and attachment heating models may be enhanced. This indicates that the synergism of the electron attachment and magnetic field has a significant effect upon the distribution function.

Figure 6.19: The percentage difference between the bulk and flux values of $n_0 D_{yy}$ (a) and $n_0 D_{zz}$ (b) as a function of $\psi$ for $B/n_0$ of 100, 200 and 500 Hx for the modified attachment model of Ness and Robson.

In order to demonstrate the explicit effects of the electron attachment on the diagonal elements of the diffusion tensor, in figures 6.19 (a) and (b) the percentage difference between the bulk and flux values of $n_0 D_{yy}$ and $n_0 D_{zz}$ is shown. As for the ionization model of Lucas and Saelee, we chose $B/n_0$ of 100, 200 and 500 Hx and $\Delta$ is given as a function of $\psi$. In contrast to the
ionization model of Lucas and Saelee, we observe that $\Delta$ assumes both the positive and negative values. For the attachment cooling model and for $n_0D_{yy}$, $\Delta$ is less than zero for all $B/n_0$ and $\psi$. Thus the bulk component is less than the flux component for all $B/n_0$ and $\psi$. In addition, the bulk component decreases when the amplitude of the electron attachment cross section increases. On the other hand, for the attachment heating model and for $n_0D_{yy}$, $\Delta$ assumes the positive values. Thus the bulk is greater than its flux component. This indicates that the decrease in electron numbers due to attachment may lower or enhance diffusion along the $y$-direction depending on the energy dependence of the attachment cross section. In particular, for $B/n_0$ of 1000 Hx there is a range of $\psi$ where the opposite situation occurs but we believe that this is rather a sign of deterioration in the convergence of the bulk component.

In contrast to $n_0D_{yy}$, the bulk corrections associated with the $n_0D_{zz}$ assumes both the positive and negative values for the attachment cooling model. In the range $0 - 45^\circ$ $\Delta$ is positive independently of $B/n_0$, indicating that the bulk is greater than the flux component. This trend proceeds further when increasing $\psi$ for $B/n_0$ of 100 Hx while for $B/n_0$ of 200 and 500 Hx the opposite situation occurs: the bulk is less than its flux component. For the attachment heating model we observe that bulk are less than their flux components for $B/n_0$ of 100 and 200 Hx and for all $\psi$.

Figure 6.20: Variation of the off-diagonal elements $D_{xy}, D_{yx}, D_{xz}, D_{zx}$ as a function of $B/n_0$ and $\psi$ for the modified attachment model of Ness and Robson for the same conditions as in Fig. 6.13.
6.4.4 Off-diagonal elements of the diffusion tensor

In this section we show the variation of the off-diagonal elements of the diffusion tensor with $B/n_0$ and $\psi$. In figures 6.20 and 6.21 we show the off-diagonal elements of the diffusion tensor as a function of $B/n_0$ and $\psi$. As already remarked, these transport properties generally satisfy the symmetry properties outlined by White et al. (1999a), independently of the gas considered. From figures 6.20 and 6.21 we observe that the implicit effect of the electron attachment on the off-diagonal elements is dependent on the energy dependence of the attachment cross section, $B/n_0$ and $\psi$. While for the attachment cooling model the off-diagonal diffusion coefficients are decreasing functions of both the amplitude of the electron attachment cross section and $B/n_0$, for the attachment heating model these transport quantities are enhanced by the action of the electron attachment. Once more it is important to note that these diffusion coefficients can have the magnitudes of equivalent order to those of diagonal elements of the diffusion tensor. As a consequence, the off-diagonal elements should be considered in fluid modeling of plasma discharges.

6.4.5 The diagonal elements of the temperature tensor

In figure 6.22 we show the variation of the diagonal elements of the temperature tensor with $B/n_0$ and $\psi$. As can be observed, the variation of these transport properties with $B/n_0$ and $\psi$ is qualitatively the same as that of the mean energy. For both the attachment cooling and attachment heating models the diagonal elements of the diffusion tensor are monotonically decreasing functions of $B/n_0$ and/or $\psi$ which is a clear indication of the cooling action associated with an increasing perpendicular (to $E$) component of $B$. The weak anisotropic nature of the temperature tensor is clearly evident from figure 6.22. Note that a weak anisotropy of the temperature tensor reflects the weak anisotropy of the velocity distribution function. Significant inelastic processes are in general required to generate significant anisotropy in the temperature...
tensor and hence these attachment model gases are not good candidates for such studies. Better option would be the modification of these models or employing the Reid ramp model modified with non-conservative cross sections.

Figure 6.22: Variation of the diagonal elements of the temperature tensor as a function of $B/n_0$ and $\psi$ for the modified attachment model of Ness and Robson for the same conditions as in Fig. 6.13.

6.5 Two term approximation vs multi-term calculations and validity of Legendre polynomial expansions

The aim of this section is to study the convergence trends in the $l$- and $m$-indices as a function of $E/n_0$ and $\psi$. For illustrative purpose, we restrict our discussion to the ionization model of Lucas and Saelee. The model parameter $F$ is set to 0.5 and hence the cross sections for electronic excitation and ionization have the same magnitude. In order to enhance the significance of inelastic collisions, we perform calculations for $E/n_0$ of 100 and 200 Td. The $B/n_0$ is set to 1000 Hx and all quantities are presented as a function of $\psi$. The convergence in the $l$- and $m$-indices is treated independently. The convergence trends and rates in the $\nu$-index are a function of basis temperature $T_b$ (for a given mass ratio). A smoothly varying convergence in the $\nu$-index is achieved through the careful selection of a $T_b$ as $E/n_0$ and/or $\psi$ are modified. Hence the convergence trend in the $\nu$-index is not presented and the focus is solely on the convergence trends in the $l$- and $m$-indices. In what follows, we highlight the way in which convergence is achieved in one index after having obtained convergence in the other two indices. The convergence is analyzed by considering the difference between results for the transport coefficients/properties obtained by a multi-term Boltzmann analysis and approximations of interest.

To study in detail the convergence in the $l$ and $m$ indices, a comprehensive investigation of the velocity distribution function (including its visualization) is inevitable. By doing so, one may establish connection between the convergence trends and variations in the anisotropy of
the distribution function. This was the program of White and co-workers who considered the convergence trends for electrons in methane (White et al., 1999d) and for electrons in carbon dioxide and ions in model gases (White, 2001). Such program is beyond the scope of this work. However, in this work we present and highlight some interesting points associated with the influence of ionization on the convergence trends.

The convergence of the $l$-index (e.g. the convergence of the spherical harmonics expansion) is dependent on the dominant types of collisional process present. As pointed out many times by Robson and co-workers (see for example Ness and Robson (1986), Ness (1994), White et al. (2003)) the two-term approximation is sufficient to ensure accuracies of 2% or less only for gases with elastic collisional processes only. Whenever inelastic collisions are present, the large energy exchange in collisions is responsible for the development of anisotropy in the velocity distribution function and hence one may never be sure about the accuracy of the two-term approximation. In this context, for atomic systems and for the low values of $E/n_0$ it has been anticipated that the two-term approximation is of sufficient accuracy. However, it must be emphasized that it is exception, more than the rule, that the two-term approximation is sufficient.

To illustrate the failure of the two-term approximation for the ionization model of Lucas and Saelee, in figure 6.23 we display the percentage differences between the two-term and multi-term values for the mean energy, ionization rate and $z$-component of the gradient energy vector as a function of $\psi$ for the ionization model of Lucas and Saelee (black line: $E/n_0 = 100$ Td; red line: $E/n_0 = 200$ Td).

![Figure 6.23: The percentage difference between two-term and multi-term results for the mean energy, ionization rate and $z$-component of the gradient energy vector as a function of $\psi$ for the ionization model of Lucas and Saelee (black line: $E/n_0 = 100$ Td; red line: $E/n_0 = 200$ Td).](image)

To illustrate the failure of the two-term approximation for the ionization model of Lucas and Saelee, in figure 6.23 we display the percentage differences between the two-term and multi-term values for the mean energy, ionization rate and $z$-component of the gradient energy vector as a function of $\psi$. Likewise, in figures 6.25-6.27 the percentage differences between the two-term and multi-term values for the drift velocity components (both the bulk and flux), diagonal elements of the diffusion tensor (both the bulk and flux) and diagonal elements of the temperature tensor are shown as a function of $\psi$. The $l_{\text{max}} = 5$ was required to achieve 0.5% accuracy for all transport coefficients and properties. The inadequacy of the two-term approximation for all transport coefficients and properties is clearly evident. We observe that different transport coefficients

141
show different convergence trends and have different rates of convergence. From figure 6.23 we observe that the mean energy and ionization rate have errors less than 10% while the z-component of the gradient energy vector has errors of the order of 30%. Generally speaking, the errors associated with these transport quantities are a decreasing function of $\psi$. For the ionization model of Lucas and Saelee we must bear in mind that the number of $l$ terms required for convergence of the transport coefficients/properties increases with swarm mean energy, as the inelastic processes start to play more important role. For fixed values of $E/n_0$ and $B/n_0$, the mean energy decreases as $\psi$ increases. Hence one would expect the convergence of the $l$ index to improve as $\psi$ increases. This is a clear sign that the anisotropy in the velocity distribution function decreases for an increasing $\psi$. On the other hand, as $E/n_0$ increases from 100 to 200 Td the errors are enhanced. This appears to reflect the general trend for the ionization model of Lucas and Saelee to enhance the anisotropy of the velocity distribution function as $E/n_0$ increases. In the limit of perpendicular fields, we observe small but noticeable decrease in the accuracy of the two-term results for the mean energy and z-component of the gradient energy vector. In case of the mean energy, these differences are within the accuracy tolerance of 0.5%. While the two-term results for the mean energy and ionization rate generally tend to overestimate the corresponding multi-term resuls, the two-term results for the z-component of the gradient energy vector generally underestimate the corresponding multi-term results.

![Figure 6.24](attachment:image.png)

Figure 6.24: The percentage difference between two-term and multi-term results for the drift velocity components as a function of $\psi$ for the ionization model of Lucas and Saelee. The solid lines represent the flux values while the dashed lines represent the bulk values (black line: $E/n_0 = 100$ Td; red line: $E/n_0 = 200$ Td).

The errors between the two-term and multi-term results for the bulk and flux drift velocity components are displayed in figure 6.24. We observe that the errors between the two-term and multi-term results for the flux values of the drift velocity components are a decreasing function of $\psi$ and an increasing function of $E/n_0$. The flux drift velocity components along $y$- and $z$-directions can have the errors of the order of 10% while the drift velocity component along the
The errors between the two-term and multi-term results for the bulk components of both \( W_y \) and \( W_z \) are significantly less than the corresponding errors associated with the flux components. The errors associated with the bulk \( W_y \) are within 1% for both \( E/n_0 \) of 100 and 200 Td while the errors associated with the bulk \( W_z \) are within 1% for \( E/n_0 \) of 100 Td and 2% for \( E/n_0 \) of 200 Td, respectively. On the other hand, the errors between the two-term and multi-term results for the bulk component of \( W_x \) are significantly larger than the corresponding errors associated with the flux values.

Figure 6.25: The percentage difference between two-term and multi-term results for the diagonal elements of the diffusion tensor as a function of \( \psi \) for the ionization model of Lucas and Saelee. The solid lines represent the flux values while the dashed lines represent the bulk values (black line: \( E/n_0 = 100 \) Td; red line: \( E/n_0 = 200 \) Td).

The errors between the two-term and multi-term results for the bulk and flux components of the diagonal elements of the diffusion tensor are displayed in figure 6.25. The differences between the two-term and multi-term results for both the bulk and flux components of the diagonal elements of the diffusion tensor show complex dependencies with respect to \( \psi \). Generally speaking, the errors between the two-term and multi-term results for the flux components of \( n_0D_{xx} \) and \( n_0D_{zz} \) are a decreasing function of \( \psi \) and an increasing function of \( E/n_0 \). The maximum errors between the two-term and multi-term results for both the bulk and flux components of \( n_0D_{yy} \) are in the limit of parallel fields.

These results clearly show that obtaining general convergence properties is difficult even for such simple model gas system. One may expect more difficulties in understanding convergence properties associated with real gases (see for example White et al. (1999d)). In general, however, one may conclude that the closer the distribution is to a spherically symmetric distribution the better the accuracy of the two-term approximation and in general the quicker convergence. Hence as \( \psi \) is increased, we generally observe a reduction in the error associated with the two-term approximation. This applies for both the bulk and flux components of the transport coefficients.
Figure 6.26: The percentage difference between two-term and multi-term results for the diagonal elements of the temperature tensor as a function of $\psi$ for the ionization model of Lucas and Saelee (black line: $E/n_0 = 100$ Td; red line: $E/n_0 = 200$ Td).

Figure 6.27: The percentage difference between results for the mean energy, ionization rate and $z$-component of the gradient energy vector obtained for the $m_{\text{max}} = 1$ and 5 truncation ($l_{\text{max}} = 5$) as a function of $\psi$ for the ionization model of Lucas and Saelee (black line: $E/n_0 = 100$ Td; blue line: $E/n_0 = 200$ Td).

The consideration of the convergence in the $m$-index is of great importance from a computational point of view. Truncation of the $m$ summation dramatically reduces the size of the coefficient matrix and hence decreases the computational time. In what follows, a value of $l_{\text{max}} = 5$ was chosen, while the $m$-index was incremented up to $l_{\text{max}}$. A value of $m_{\text{max}} = 0$ represents a Legendre polynomial expansion. Generally speaking, the Legendre polynomial expansion procedure for solving the Boltzmann equation is inadequate for determining transport properties perpendicular to the vector of electric field. In figures 6.27-6.30 we display the percentage
difference between results for transport coefficients/properties obtained for the $m_{\text{max}} = 1$ and 5 truncation ($l_{\text{max}} = 5$) as a function of $\psi$. We observe that different transport coefficients have different rates and trends of convergence. Convergence in the $m$-index is rapid for parallel fields with $m_{\text{max}} = 1$ to achieve accuracy of 0.5%. Likewise, the convergence in the $m$-index is rapid for some transport coefficients/properties in the limit of perpendicular fields with $m_{\text{max}} = 1$ to achieve accuracy of 0.5%. These include the $\varepsilon$, $k_{\text{ion}}$, $W_x$, $W_z$ and $n_0D_{xx}$ at $E/n_0$ of 100 and 200 Td. It should be noted that this applies for both the bulk and flux transport coefficients. Similar trends can be observed for the temperature tensor components at $E/n_0$ of 100 Td. Generally speaking, we may observe a tendency for the $m$-index to be less important in the limit of perpendicular fields. Intuitively one would expect this as the number of $l$ terms required for convergence is significantly reduced in the limit of perpendicular fields for $E/n_0$ and $B/n_0$ considered in this work.

![Graph showing the percentage difference between results for drift velocity components](image)

Figure 6.28: The percentage difference between results for the drift velocity components obtained for the $m_{\text{max}} = 1$ and 5 truncation ($l_{\text{max}} = 5$) as a function of $\psi$ for the ionization model of Lucas and Saelee. The solid lines represent the flux values while the dashed lines represent the bulk values (black line: $E/n_0 = 100$ Td; blue line: $E/n_0 = 200$ Td).

As for the Reid’s model (White et al., 1999a), the presented results suggest that the dependence upon the $m$-index increases as $\psi$ increases from weak to moderate. For the present work a moderate $\psi$ corresponds to a range between 40 and 75 degrees. In the limit of perpendicular fields anisotropy in the velocity space is significantly diminished and $m_{\text{max}} = 2$ is generally required to ensure the accuracy of 0.5% for all transport coefficients/properties. Therefore, the dependence upon the $m$-index generally displays some maximal property with $\psi$. As $E/n_0$ increases, the percentage differences between results obtained for the $m_{\text{max}} = 1$ and 5 truncation ($l_{\text{max}} = 5$) are enhanced and consequently the maximal property in the $m$ dependence becomes more pronounced.
Figure 6.29: The percentage difference between results for the diagonal elements of the diffusion tensor obtained for the \( m_{\text{max}} = 1 \) and 5 truncation \( (l_{\text{max}} = 5) \) as a function of \( \psi \) for the ionization model of Lucas and Saelee. The solid lines represent the flux values while the dashed lines represent the bulk values (black line: \( E/n_0 = 100 \) Td; blue line: \( E/n_0 = 200 \) Td).

Figure 6.30: The percentage difference between results for the diagonal elements of the temperature tensor obtained for the \( m_{\text{max}} = 1 \) and 5 truncation \( (l_{\text{max}} = 5) \) as a function of \( \psi \) for the ionization model of Lucas and Saelee (black line: \( E/n_0 = 100 \) Td; blue line: \( E/n_0 = 200 \) Td).