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THE MULTI-TERM BOLTZMANN EQUATION ANALYSIS AND MONTE CARLO STUDY OF HYDRODYNAMIC AND NON-HYDRODYNAMIC CHARGED PARTICLE SWARMS

Thesis submitted by
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in February 2009

for the degree of Doctor of Philosophy
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Saša Dujko,

27 February 2009.

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Abstract

The progress and further improvement of modern technology associated with the non-equilibrium magnetized plasma discharges require the most accurate modeling of charged particle transport under the influence of electric and magnetic fields in neutral gases. It is the aim of this Thesis to present a theoretical and numerical investigation of hydrodynamic and non-hydrodynamic charged particle swarms in neutral gases under the influence of dc and ac electric and magnetic fields with applications of non-equilibrium magnetized plasma discharges to plasma processing, gas laser discharges and drift chambers for detection particles in mind. Two complimentary techniques are developed: A time-dependent true multi-term solution of Boltzmann's equation and a Monte Carlo simulation technique, both adapted to consider both time-dependent hydrodynamic and steady state non-hydrodynamic conditions. The accuracy and generality of both techniques are established in their application to benchmark systems (existing and developed as part of the thesis) as well as the application to real gaseous systems.

Binary elastic, inelastic and non-conservative (attachment and electron impact ionization) collisions between the swarm particles and neutral gas molecules are considered. The angular dependence of the phase space distribution function in velocity space is represented in terms of an expansion in spherical harmonics. No restrictions are placed on the number of spherical harmonics in the polynomial expansion nor on the space and time-dependence of the phase space distribution function. In addition, there are no restrictions on the mass ratio between the swarm particle and neutral gas molecule (e.g., the present formalism is equally valid for electrons and ions) nor on the neutral gas temperature and cross sections. The speed dependence of the phase space distribution function is represented by an expansion in Sonine polynomials about a Maxwellian distribution function using a well-known two-temperature method. By doing so, the Boltzmann equation is decomposed into a hierarchy of coupled kinetic equations for tensorial expansion coefficients.

For time-dependent hydrodynamic regime, the space dependence of the phase space distribution function is represented in terms of powers of density gradient operator. A second order density gradient expansion was required to highlight the explicit modification of transport coefficients about by non-conservative collisional processes of attachment and electron impact ionization. Employing the implicit finite difference scheme for evaluation of the time-derivatives, the Boltzmann equation under conditions of time-dependent hydrodynamic regime is transformed into a hierarchy of doubly infinite coupled inhomogeneous matrix equations for the time-dependent moments. Truncation of both the Sonine polynomials and spherical harmonics results in a sparse system of coupled complex equations. This system of equations is solved using standard sparse inversion routines.

Under non-hydrodynamic conditions (such as those found in an idealized steady-state Townsend (SST) experiment) a density gradient expansion procedure is not valid and the space dependence of the phase space distribution function is retained explicitly throughout the entire decomposition process of the Boltzmann equation. For numerical discretization in configuration space the finite difference scheme and pseudo-spectral method are employed. Boundary conditions are

specified for swarms undergoing conservative collisions only and techniques for solving the resulting large system of algebraic complex equations are discussed. The explicit effects of ionization and attachment on the spatially resolved electron transport properties under non-hydrodynamic conditions are investigated by a Monte Carlo simulation technique. In particular, we identify the relations for the conversion of hydrodynamic transport properties to those found in an idealized steady-state Townsend experiment. Our Monte Carlo simulation code and sampling techniques appropriate to these experiments have provided us with a way to test these conversion formulae and their convergence.

For swarms moving in an unbounded gas under hydrodynamic conditions when non-conservative collisions are operative, we focus on two situations: (i) temporal relaxation of the electrons in dc electric and magnetic fields crossed at arbitrary angle; and (ii) time-dependent behavior of electron swarms in ac electric and magnetic fields crossed at arbitrary angle and at arbitrary phase difference. There are no restrictions on the field amplitudes nor on the frequency of the applied electric and magnetic fields. Recent studies on the temporal relaxation of electrons in gases are extended by overcoming the inherent inaccuracies of the two-term approximation for solving the Boltzmann equation and by addressing the temporal relaxation of spatial inhomogeneities through a study of the diffusion tensor. In the framework of ac studies, the variation of the electron transport coefficients with electric and magnetic field strengths, field frequency, phase difference between the fields and angle between the fields is addressed using physical arguments for certain model and real gases. A multitude of kinetic phenomena were observed 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. Most notably, a proposed new mechanism for collisional heating in inductively coupled plasmas has emerged from this thesis. It is shown that the synergism of temporal non-locality and cyclotron resonance effect under conditions of time-dependent, high frequency electric and magnetic fields can be used to pump the energy into the swarm. In particular, it is demonstrated that the magnetic field amplitude, phase-difference between the fields and field frequency can be tuned to exploit/control this phenomenon.

The synergism of magnetic field and non-conservative collisions on spatial relaxation of a swarm of charged particles in an idealized SST experiment is investigated. Results are presented for electrons in varying configurations of dc electric and magnetic fields for certain model and real gases. It is found that the spatial relaxation characteristics including the type of relaxation (monotonic/oscillatory), the relaxation length and period of oscillations can be controlled either by the variation of the magnetic field strengths or by the angles between the fields.

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