Electron swarm kinetics in electric and magnetic fields crossed at arbitrary angles

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The LisbOn KInetics Monte Carlo (LoKI-MC) code, to be soon released as open-source, solves the steady-state electron kinetics in any complex gas mixture under constant electric fields. This work extends its capability to alternated electric fields and to constant magnetic fields crossed at arbitrary angles. The integration of the equations of motion during the electron free flights is performed analytically, avoiding the computational overload in conditions of strong magnetic fields that the usual “Boris rotation” method suffers. The code is verified against benchmark calculations available in the literature.

Low-temperature plasmas (LTPs) are strongly reactive systems, characterized by a low ionization degree, high electron temperature and heavy-species translational temperature close to the room temperature. The strong non-equilibrium of LTPs can efficiently stimulate several chemical processes relevant for industrial, medical and environmental applications. Electrons play a major role in these plasmas, since they are responsible for transmitting the energy acquired from the electric field to the heavy particles through various collisional channels. Therefore, the control of the energy distribution of the electrons is essential to maximize the capability of LTPs.

The electron kinetics in gas discharges can be described in detail by solving numerically the differential electron Boltzmann equation (EBE), or by tracking the stochastic motion of the individual electrons using Monte Carlo methods. Publicly available solvers based on either approach were developed in the last decades, for the benefit of the LTP community. However, most of them are based on the low-anisotropy approximation to solve the EBE, keeping only two terms in an expansion of the electron distribution function in Legendre polynomials over the velocity space, and/or do not allow the simulation of complex gas mixtures, with electronic, vibrational and rotational states.

In a previous work, we presented the LisbOn Kinetics Monte Carlo (LoKI-MC) solver, to be published soon as open source, that addresses the simulation of the steady-state electron kinetics in any complex gas mixture of atomic/molecular species, describing electron collisions with any target state, and accounting for superelastic and stepwise excitation processes, subject to a constant electric field [1]. Since the Monte Carlo approach does not rely on the two-term approximation, LoKI-MC provides an accurate description for an arbitrarily high reduced electric field, E/N. Here, we generalize the formulation to a high-frequency (HF) electric field, $\mathbf{E}$, together with a constant magnetic field, $\mathbf{B}$, with an arbitrary direction.

Typically, Monte Carlo studies of electron swarms under a magnetic field employ the “Boris rotation” method [2,3] to propagate the electrons during the free-collision flights, which is computationally simple and easily applicable in configurations of non-uniformity in space. This algorithm is constructed so as to preserve the Larmor rotation of electrons in conditions of null electric field. To assure a good numerical convergence, the time-steps must be significantly smaller than the gyro time, leading to a severe drawback when the magnetic field is strong. Here, we take advantage of the space uniformity in our formulation and solve analytically the electron motion under the fields **E** and **B**. This approach eliminates the restriction in the time-steps associated to the magnetic field. Thus, the computational efficiency of the temporal evolution of the system is only ruled by the electron collision frequencies, as in the case of null magnetic field.

To validate our implementation, we compare LoKI-MC calculations with the results of previous works, obtained using two models with analytical cross sections: Reid [4] and Lucas-Saelee [5]. In both cases, there is a remarkable agreement with the literature [2,3]. Figures 1 and 2 exemplify the excellent concordance with [2] for the calculation of the electron mean energy and diffusion coefficient in the Reid model, which is characterized by a constant elastic cross section and an excitation cross section increasing linearly with energy. In these calculations the electric field is perpendicular to the magnetic field, the reduced electric field E/N is fixed to 12 Td, and the reduced magnetic field B/N is varied from 0 to 500 Hx, where 1 Hx = 10^{-27} T m^3. In the conference, the comparison will be extended and the physical effects of the magnetic field on the swarm parameters will be discussed. Moreover, the influence of the magnetic-field angle will be analyzed in the Lucas-Saelee model and benchmarked with the results of Dujko *et al* [3]. Finally, we will investigate electron swarms in real gases, such as argon and oxygen.

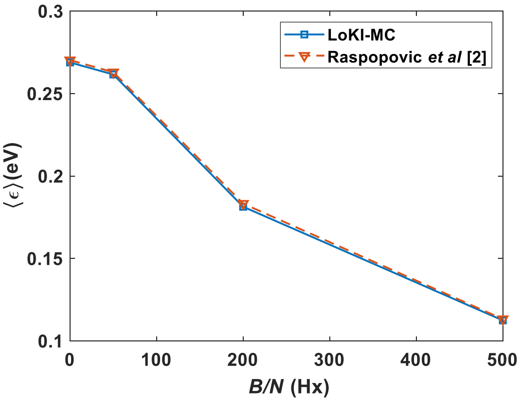

Figure 1: Electron mean energy using the Reid model.

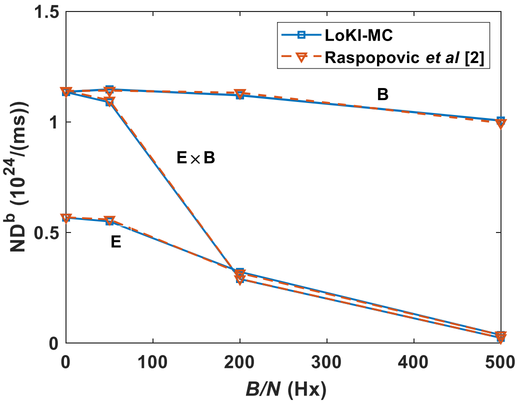

Figure 2: Bulk diffusion coefficients along various directions, using the Reid model.

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