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A numerical solver for the homogeneous Boltzmann Equation

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In this work we present some results from a numerical solution of the homogeneous electron Boltzmann equation (EBE) for electrons in an uniform electric field, using the classical two term expansion. This EBE solver was specially designed to be used as part of global models for low temperature plasmas. It accounts for oscillating fields, electron-neutral collisions and electron-electron collisions. In order to validate the EBE solver, we compare calculated transport parameters with experimental data from electron swarm experiments in N_2 and Ar.

I. INTRODUCTION

The electron energy distribution function (EEDF) plays a key role on the theoretical description of low temperature plasmas. In general, it is not always possible to assume a Maxwellian distribution and the EEDF deviates considerably from equilibrium. In these cases, one possible approach is to calculate the EEDF by solving the electron Boltzmann equation (EBE) [1].

In this work, we present the results of a numerical solver of the homogeneous electron Boltzmann equation in the *two term expansion in spherical harmonics approximation*. This solver was designed to work with any kind of gas composition, as long as a consistent set of electron-neutral collision cross sections is given. In order to validate the EBE solver, we compared the calculated electron mobility and characteristic energy with experimental data from electron swarm experiments in N_2 and Ar.

II. BOLTZMANN EQUATION

The isotropic component of the homogeneous EBE ($f(u)$, with the normalization $\int_0^\infty f(u)\sqrt{u}\,du = 1$) can be written as a continuity equation of the total power flux $G(u)$, which is the sum of the fluxes driven by the applied electric field, G_E, elastic collisions with the atoms, G_c, and electron-electron collisions, G_{ee}

$$\begin{aligned}\frac{dG}{du} &= \frac{d}{du}\left(G_E + G_{ee} + G_c\right) \\ &= \sum_{s,j} n_s \left[(u+u_j)\delta_0\sigma_j^s(u+u_j)f(u+u_j) - u\delta_0\sigma_j^s(u)f(u) + \right. \\ &\qquad \left. (u-u_j)\delta_j\sigma_j^{'s}(u-u_j)f(u-u_j) - u\delta_j\sigma_j^{'s}(u)f(u)\right] \quad (1)\end{aligned}$$

where n_s is the concentration of specie s, u_j is the excitation or ionization threshold, σ_j^s is the cross section of the inelastic electron collision in which the target particle is excited from the ground to an excited state j, $\sigma_j^{'s}$ is the cross section of the reverse process (*superelastic collision*) and δ_j is the population of heavy particles in state j. The electron energy u is given in units of electronvolts. The fluxes driven by the applied electric field, G_E and elastic collisions with the atoms, G_c, are given by

$$G_E = -\frac{2e}{3m}\frac{\nu_c(u)}{\nu_c^2+\omega^2}E^2u^{3/2}\frac{df}{du}\,, \quad (2)$$

$$G_c = -N\sqrt{\frac{2e}{m}}\left(\sum_s \frac{2m}{M_s}\delta_s\sigma_m^s\right)u^2\left(f + T_0\frac{df}{du}\right)\,, \quad (3)$$

where N is the number density of heavy particles, σ_m^s and M_s are the total momentum transfer cross section and the mass of the neutral specie s, T_0 is the gas temperature in eV and $\nu_c(u)$ is the colision frequency, given by

$$\nu_c(u) = \sqrt{\frac{2e}{m}}N\sum_s \delta_s u^{1/2}\sigma_m^s\,. \quad (4)$$

The energy flux due to *e-e* interactions, G_{ee}, is given by

$$G_{ee} = -8\pi\left(\frac{e^2}{4\pi\varepsilon_0 m}\right)^2\frac{\ln\Lambda}{v^3}n_e u^{3/2}\left[I(u)f + J(u)\frac{df}{du}\right]\,, \quad (5)$$

where

$$I(u) = \int_0^u f\sqrt{x}\,dx\,; \quad J(u) = \frac{2}{3}\left(\int_0^u fx^{3/2}dx + u^{3/2}\int_u^\infty f\,dx\right)\,, \quad (6)$$

where $\ln\Lambda$ is the Coulomb logarithm. Rotational collisions were taken into account in the continuous approach proposed by Frost and Phelps [2].

Equation 1 can be solved numerically by converting it into a set of equations by finite differencing the electron energy variable [3]. If electron-electron collisions are not taken into account, the system reduces to a set of linear equations and can be easily solved: otherwise, the set of non-linear equations must be solved by an iterative procedure.

A computer code was written in MATLAB® in order to solve this numerical problem. It takes as input all the relevant physical parameters, such as temperature, pressure, reduced electric field, oscillation field frequency, ionization degree, gas composition and electron-neutral collision cross sections, and also some numerical parameters, such as the number of cells in the energy grid and the upper limit of integration in energy space.

III. RESULTS AND DISCUSSION

Figures 1 and 2 compare experimental measurements and theoretical results for the characteristic energy and electron reduced mobility in N_2 and Ar. The reduced mobility is defined as the quotient between the drift velocity (mean velocity), v_d, and the reduced electric field, E,

$$\mu \times N = \frac{v_d}{E} \times N = -\frac{1}{3}\sqrt{\frac{2e}{m_e}} \int_0^\infty \frac{u}{\sum_s \delta_s \sigma_m^s} \frac{df}{du} du \,, \quad (7)$$

where e is the elementary charge and m_e is the electron mass. The characteristic energy is defined as the ratio between the free diffusion coefficient, D_0, and the electron mobility

$$\varepsilon_c = \frac{D_0}{\mu} = \frac{1}{3\mu N}\sqrt{\frac{2e}{m_e}} \int_0^\infty \frac{u f(u)}{\sum_s \delta_s \sigma_m^s} du \,. \quad (8)$$

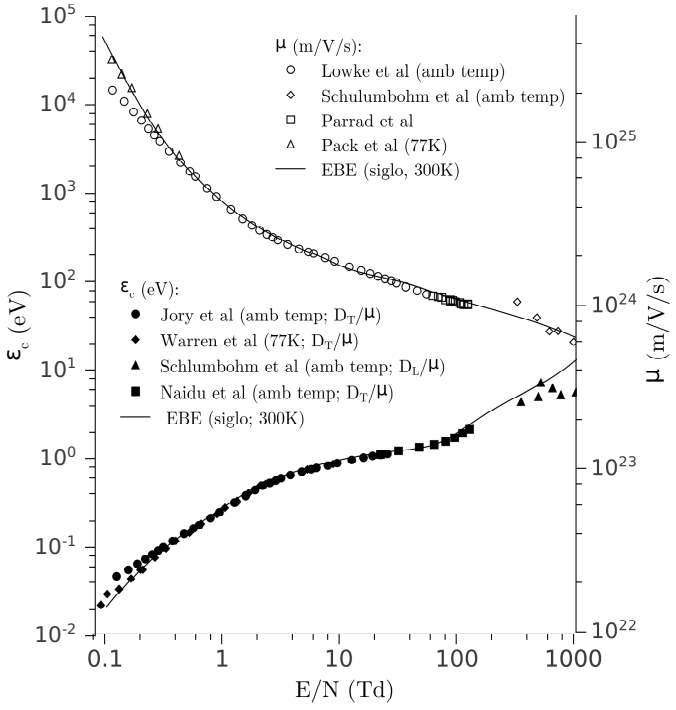

Figure 1: Characteristic energy and electron reduced mobility in N_2: experimental [4] and theoretical values. The set of cross sections (siglo) was extracted from *LXCat* database [4].

Overall, there is an excellent agreement between the calculated values and the experimental results. However, there are small discrepancies in the case of N2 for the lower values of the reduced electric field. The reason of that discrepancy is the failure of the continuous approximation to describe the effect of rotational collisions in the lower range of reduced electric field when the temperature is not low enough to satisfy the assumptions made by Frost and Phelps [2]. We tested this hypothesis by considering the first 25 rotational transitions on the right-hand side of equation 1 and found good agreement with experiment.

IV. ACKNOWLEDGEMENTS

One of the authors, M. A. R., acknowledges a PhD fellowship from CNPq which enabled him to carry out this work.

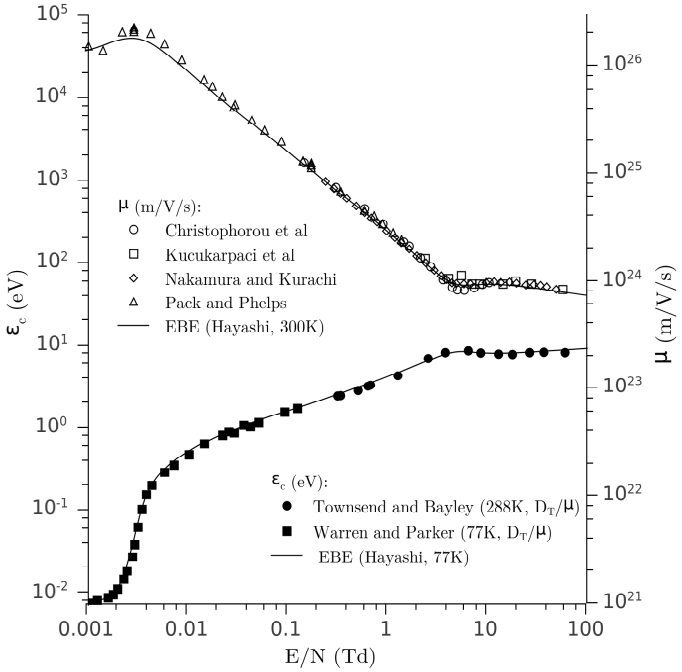

Figure 2: Characteristic energy and electron reduced mobility in Ar: experimental [4] and theoretical values. The set of cross sections (Hayashi) was extracted from *LXCat* database [4].

[1] Alves L L, Gousset G and Ferreira C M 1992 *J. Phys. D: Apply. Phys.* **25** 1713–1732
[2] Frost L S and Phelps A V 1962 *Physical Review* **127** 1621–1633
[3] Rockwood S D 1973 *Physical Review A* **8** 2348–2358
[4] LXCat 2011 Electron scattering database retrieved October 17, 2011 URL `http://www.lxcat.laplace.univ-tlse.fr`