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Simulation of Bipolar Charge Transport in Graphene by Using a Discontinuous Galerkin Method

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Abstract. Charge transport in suspended monolayer graphene is simulated by a numerical deterministic approach, based on a discontinuous Galerkin (DG) method, for solving the semiclassical Boltzmann equation for electrons. Both the conduction and valence bands are included and the interband scatterings are taken into account.

The use of a Direct Simulation Monte Carlo (DSMC) approach, which properly describes the interband scatterings, is computationally very expensive because the valence band is very populated and a huge number of particles is needed. Also the choice of simulating holes instead of electrons does not overcome the problem because there is a certain degree of ambiguity in the generation and recombination terms of electron-hole pairs. Often, direct solutions of the Boltzmann equations with a DSMC neglect the interband scatterings on the basis of physical arguments. The DG approach does not suffer from the previous drawbacks and requires a reasonable computing effort.

In the present paper the importance of the interband scatterings is accurately evaluated for several values of the Fermi energy, addressing the issue related to the validity of neglecting the generation-recombination terms. It is found out that the inclusion of the interband scatterings produces huge variations in the average values, as the current, with zero Fermi energy while, as expected, the effect of the interband scattering becomes negligible by increasing the absolute value of the Fermi energy.

AMS subject classifications: 82D37, 82C70, 65M60, 82C80

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1 Introduction

The last years have witnessed a great interest in 2D-materials for their promising applications. The most investigated one is graphene which is considered as a potential

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new semiconductor material for future applications in nano-electronic [1–4] and opto-electronic devices [5]. A reasonable and physically accurate model for charge transport is based on semiclassical Boltzmann equations (quantum effects have also been included in the literature, e.g. see [6,7]). Usually, the available solutions have been obtained by direct Monte Carlo simulations, e.g. a new Direct Simulation Monte Carlo (DSMC) procedure has been devised in [8–10] in order to properly take into account the Pauli exclusion principle. Direct solutions of the electron transport equations with finite difference methods have been obtained in [3] while a Discontinuous Galerkin (DG) method has been used in [8, 11, 12]. See [13, 14] for application of the DG method to traditional semiconductors, while numerical schemes for the Wigner equation can be found in [15]. A hydrodynamical model based on the maximum entropy principle (MEP) has been formulated in [16] using a set of field variables which proved to be successful for traditional semiconductors as silicon [17–23], gallium arsenide [17, 24], silicon carbide [25]. In general both electrons in the conduction and valence bands contribute to charge transport in graphene and the zero gap energy band allows for the creation of electron-hole pairs by scattering with phonons around the Dirac points. Therefore, one has also to include interband electron-phonon scatterings. However, if a gate voltage is applied, it is possible to modify the value of the Fermi energy ε_F creating a kind of doping as in conventional semiconductors. If ε_F is positive and high enough, one has a kind of n-doping and the only relevant contribution to the current is due to the electrons in the conduction band. Analogously, if $\varepsilon_F < 0$ one has a kind of p-doping. The use of DSMC in the bipolar case is rather heavy from a computational point of view because the valence band is very populated and a huge number of simulation particles is needed. A viable way to overcome the problem could be to simulate, in the valence band, holes instead of electrons. Unfortunately, this introduces a certain degree of ambiguity in the generation and recombination terms of electron-hole pairs and makes the approach rather questionable, as explained in the next section. For such a reason, often the interband scattering is neglected. The DG method does not suffer from the previous difficulties and keeps the computational effort to a reasonable level. In the present paper, by performing an extensive numerical simulation with the DG method of the system of Boltzmann equations for electrons in the conduction and valence bands, the importance of the interband scatterings is accurately evaluated for several values of the Fermi energy in the case of suspended monolayer graphene under a constant external electric field. It is addressed the issue related to the validity of neglecting the generation-recombination terms. It is found out that the inclusion of the interband scatterings induces huge variations in the average values, as the current, with zero Fermi energy while, as expected, the effect of the interband scatterings becomes negligible by increasing in absolute value the Fermi energy. The plan of the paper is as follows. In section 2 the semiclassical model of charge transport in graphene is recalled. In particular, there are highlighted the problems arising in the electron-hole scatterings. In section 3 the DG method, adopted in the paper, is explained. At last, in section 4 the numerical results are presented and the issue of the role played by the interband scatterings is analyzed. Some details are postponed to the Appendix.