Comparing kinetic, Monte Carlo and hydrodynamical models for electron transport in monolayer graphene

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The aim of this work is to compare, in monolayer graphene, solutions of the electron Boltzmann equation, obtained with a discontinuous Galerkin method and Monte Carlo method, with those of a hydrodynamical model based on the Maximum Entropy Principle.

1. Details

Graphene is a gapless semiconductor made of a single layer of carbon atoms arranged into a honeycomb hexagonal lattice [1]. In view of applications in graphene-based electron devices, it is crucial to understand the basic transport properties of this material.

A physically accurate model is given by a semiclassical transport equation whose scattering terms have been deeply analyzed recently [2, 3, 4]. Due to the computational difficulties, the most part of the available solutions have been obtained by direct Monte Carlo simulations. A different approach has been employed in [5].

For computer aided design (CAD) purposes, it could be useful to have macroscopic models like drift-diffusion, energy-transport and hydrodynamical ones. Macroscopic models have been proposed, for example, in [6, 7, 8].

The aim of this work is to assess the validity of the hydrodynamical model based on the Maximum Entropy Principle (MEP) [7], by comparing the solutions of this model with those of the transport equation for electrons in suspended monolayer graphene. A numerical scheme based on the discontinuous Galerkin method [9, 10] is used for finding the solutions of the electron Boltzmann equation. Also Monte Carlo simulations have performed formulating a suitable approach for taking into account the degeneracy effects without exceeding the unit for the occupation number, a problem well known in conventional semiconductor like silicon and gallium arsenide.

Comparison of the determinisic and stochastic solutions of the transport equation furnishes a cross validation of the discontinuous Galerkin approach and Monde Carlo one. Comparison of the physically average quantities, electron energy and velocity, shows that the MEP model is reasonable even if the introduction of some improvements regarding additional moments or nonlinear effects is needed.

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