Deterministic Solutions of the Transport Equation for Charge Carrier in Graphene

Armando Majorana and Vittorio Romano

Abstract The aim of this work is to use a numerical scheme based on the discontinuous Galerkin method for finding deterministic (non stochastic) solutions of the electron Boltzmann transport equation in graphene. The same methods has been already successfully applied to a more conventional semiconductor material like Si (Cheng et al., Comput Methods Appl Mech Eng 198(37–40):3130–3150, 2009; Cheng et al., Boletin de la Sociedad Espanola de Matematica Aplicada 54:47–64, 2011). A n-type doping or equivalently a high value of the Fermi potential is considered. Therefore we neglect the inter band scatterings but retain all the main electron-phonon scatterings. Simulations in graphene nano-ribbons are presented and discussed.

Keywords Charge carrier • Discontinuous Galerkin method • Electron Boltzmann equation • Electron transport

1 The Mathematical Model

Graphene is a gapless semiconductor made of a sheet composed of a single layer of carbon atoms arranged into a honeycomb hexagonal lattice [1]. In view of application 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 [2–4]. 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]. Macroscopic models can be found in [6–8].

The aim of this work is to use a numerical scheme based on the discontinuous Galerkin method for finding deterministic (non stochastic) solutions of the electron Boltzmann equation in graphene. The same methods has been already successfully applied to a more conventional semiconductor material like Si [9, 10].

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The electron energy in graphene depends on a two dimensional wave vector $\mathbf{k}$ belonging to a bi-dimensional Brillouin zone which has an hexagonal shape. The most part of electrons are in the valleys, around the vertexes of the Brillouin zone, called Dirac points or K and K' points. Usually the three K-valley are treated as a single equivalent one and similarly the three K'-valleys.

In a semiclassical kinetic setting, the charge transport in graphene is described by four Boltzmann equations, one for electrons in the valence (π) band and one for electrons in the conductions (π^*) band, that in turn can belong to the K or K' valley,

$$\frac{\partial f_{\ell,s}(\mathrm{t},\mathbf{x},\mathbf{k})}{\partial t} + \mathbf{v}_{\ell,s}\cdot\nabla_{\mathbf{x}} f_{\ell,s}(\mathrm{t},\mathbf{x},\mathbf{k}) - \frac{e}{\hbar}\mathbf{E}\cdot\nabla_{\mathbf{k}} f_{\ell,s}(\mathrm{t},\mathbf{x},\mathbf{k}) = \left.\frac{df_{\ell,s}}{dt}(\mathrm{t},\mathbf{x},\mathbf{k})\right|_{e-ph}, \qquad (1)$$

where $f_{\ell,s}(\mathrm{t},\mathbf{x},\mathbf{k})$ represents the distribution function of charge carriers in the valley ℓ (K or K'), band π or π^* ($s=-1$ or $s=1$) at position $\mathbf{x}$, time t and wave-vector $\mathbf{k}$. We denote by $\nabla_{\mathbf{x}}$ and $\nabla_{\mathbf{k}}$ the gradients with respect to the position and wave vector, respectively. The microscopic velocity $\mathbf{v}_{\ell,s}$ is related to the energy band $\varepsilon_{\ell,s}$ by

$$\mathbf{v}_{\ell,s} = \frac{1}{\hbar}\nabla_{\mathbf{k}}\,\varepsilon_{\ell,s}\,.$$

With a very good approximation [1] a linear dispersion relation holds for the energy bands $\varepsilon_{\ell,s}$ around the equivalent Dirac points; so that $\varepsilon_{\ell,s} = s\,\hbar\,v_F\,|\mathbf{k}-\mathbf{k}_\ell|$, where v_F is the (constant) Fermi velocity, $\hbar$ the Planck constant divided by 2π, and $\mathbf{k}_\ell$ is the position of the Dirac point ℓ. The elementary (positive) charge is denoted by e, and $\mathbf{E}$ is the electric field obtained by the Poisson equation, which must be coupled with the above system. The right hand side of Eq. (1) is the collision term representing the interaction of electrons with acoustic, optical and K phonons. Acoustic phonon scattering is intra-valley and intra-band. Optical phonon scattering is intra-valley and can be longitudinal optical (LO) and the transversal optical (TO); it can be intra-band, that is leaves the electron in the same band, or inter-band pushing the electron from an initial band to the other one. Scattering with optical phonon of type K pushes electrons from a valley to a neighbor one (inter-valley scattering). We assume that phonons are at thermal equilibrium. Hence, the general form of the collision term can be written as

$$\left.\frac{df_{\ell,s}}{dt}(\mathrm{t},\mathbf{x},\mathbf{k})\right|_{e-ph} = \sum_{\ell',s'}\Bigg[\int S_{\ell',s',\ell,s}(\mathbf{k}',\mathbf{k})\,f_{\ell',s'}(\mathrm{t},\mathbf{x},\mathbf{k}')\,(1-f_{\ell,s}(\mathrm{t},\mathbf{x},\mathbf{k}))\,d\mathbf{k}'$$
$$-\int S_{\ell,s,\ell',s'}(\mathbf{k},\mathbf{k}')\,f_{\ell,s}(\mathrm{t},\mathbf{x},\mathbf{k})\,\left(1-f_{\ell',s'}(\mathrm{t},\mathbf{x},\mathbf{k}')\right)d\mathbf{k}'\Bigg]$$

where the total collision term is given by the sum of the contributions of several types of scatterings

$$S_{\ell',s',\ell,s}(\mathbf{k}',\mathbf{k}) = \sum_{\nu}\left|G^{(\nu)}_{\ell',s',\ell,s}(\mathbf{k}',\mathbf{k})\right|^2\Big[\left(n^{(\nu)}_{\mathbf{q}}+1\right)\delta\left(\varepsilon_{\ell,s}(\mathbf{k})-\varepsilon_{\ell',s'}(\mathbf{k}')+\hbar\,\omega^{(\nu)}_{\mathbf{q}}\right)$$
$$+\,n^{(\nu)}_{\mathbf{q}}\,\delta\left(\varepsilon_{\ell,s}(\mathbf{k})-\varepsilon_{\ell',s'}(\mathbf{k}')-\hbar\,\omega^{(\nu)}_{\mathbf{q}}\right)\Big]\,. \qquad (2)$$

The index ν labels the νth phonon mode, $G^{(\nu)}_{\ell',s',\ell,s}(\mathbf{k}',\mathbf{k})$ is the scattering rate, which describes the scattering mechanism, due to phonons ν, between electrons belonging to valley ℓ' and band s', and electron belonging to valley ℓ and band s. The symbol δ denotes the Dirac distribution function, $\omega^{(\nu)}_{\mathbf{q}}$ the νth phonon frequency, $n^{(\nu)}_{\mathbf{q}}$ is the Bose-Einstein distribution for the phonon of type ν

$$n^{(\nu)}_{\mathbf{q}} = \frac{1}{e^{\hbar\,\omega^{(\nu)}_{\mathbf{q}}/k_B T} - 1}\,,$$

k_B is the Boltzmann constant and T the constant graphene lattice temperature. When, for a phonon ν_*, $\hbar\,\omega^{(\nu_*)}_{\mathbf{q}} \ll k_B T$, then the scattering with the phonon ν_* can be assumed elastic. In this case, we eliminate in Eq. (2) the term $\hbar\,\omega^{(\nu_*)}_{\mathbf{q}}$ inside the delta distribution and we use the approximation $n^{(\nu_*)}_{\mathbf{q}} + 1 \approx n^{(\nu_*)}_{\mathbf{q}}$.

1.1 The Model with Only One Distribution Function

In this paper we consider a numerical no stochastic technique, based on the discontinuous Galerkin method, for solving the kinetic model described in Sect. 1. In this first application, we study the case of a single distribution function f. This corresponds to a physical case, where a n-type doping or equivalently a high value of the Fermi potential is considered, and the electrons, belonging to a conduction band, do not move to the valence band. Moreover K and K' are considered equivalent. A reference frame centered in the K-point will be used. Of course, we simplify the notation, omitting the indexes s and ℓ. Now, we write the scattering rates used in our simulations, explicitly.

For acoustic phonons, usually one considers the elastic approximation, and

$$2\,n^{(ac)}_{\mathbf{q}}\left|G^{(ac)}(\mathbf{k}',\mathbf{k})\right|^2 = \frac{1}{(2\,\pi)^2}\,\frac{\pi\,D^2_{ac}\,k_B\,T}{2\hbar\,\sigma_m\,v_p^2}\,(1+\cos\vartheta_{\mathbf{k},\mathbf{k}'})\,, \tag{3}$$

where D_{ac} is the acoustic phonon coupling constant, v_p is the sound speed in graphene, σ_m the graphene areal density, and $\vartheta_{\mathbf{k},\mathbf{k}'}$ is the convex angle between $\mathbf{k}$ and $\mathbf{k}'$.

There are three relevant optical phonon scatterings: the longitudinal optical (LO), the transversal optical (TO) and the K (K) phonons. The scattering rates are

$$\left|G^{(LO)}(\mathbf{k}',\mathbf{k})\right|^2 = \frac{1}{(2\,\pi)^2}\,\frac{\pi\,D^2_O}{\sigma_m\,\omega_O}\,(1-\cos(\vartheta_{\mathbf{k},\mathbf{k}'-\mathbf{k}}+\vartheta_{\mathbf{k}',\mathbf{k}'-\mathbf{k}})) \tag{4}$$

$$\left|G^{(TO)}(\mathbf{k}',\mathbf{k})\right|^2 = \frac{1}{(2\,\pi)^2}\,\frac{\pi\,D^2_O}{\sigma_m\,\omega_O}\,(1+\cos(\vartheta_{\mathbf{k},\mathbf{k}'-\mathbf{k}}+\vartheta_{\mathbf{k}',\mathbf{k}'-\mathbf{k}})) \tag{5}$$

$$\left|G^{(K)}(\mathbf{k}',\mathbf{k})\right|^2 = \frac{1}{(2\,\pi)^2}\,\frac{2\pi\,D^2_K}{\sigma_m\,\omega_K}\,(1-\cos\vartheta_{\mathbf{k},\mathbf{k}'})\,, \tag{6}$$

where D_O is the optical phonon coupling constant, ω_O the optical phonon frequency, D_K is the K-phonon coupling constant and ω_K the K-phonon frequency. The angles $\vartheta_{\mathbf{k},\mathbf{k}'-\mathbf{k}}$ and $\vartheta_{\mathbf{k}',\mathbf{k}'-\mathbf{k}}$ denote the convex angles between $\mathbf{k}$ and $\mathbf{k}'-\mathbf{k}$ and between $\mathbf{k}'$ and $\mathbf{k}'-\mathbf{k}$, respectively.

2 The Numerical Method

We look for spatially homogeneous solutions to Eq. (1) with a constant electric field. Now, the Boltzmann equation reduces to

$$\frac{\partial f(\mathrm{t},\mathbf{k})}{\partial t} - \frac{e}{\hbar}\,\mathbf{E}\cdot\nabla_{\mathbf{k}} f(\mathrm{t},\mathbf{k}) = \int S(\mathbf{k}',\mathbf{k}) f(\mathrm{t},\mathbf{k}')\,(1-f(\mathrm{t},\mathbf{k}))\,d\mathbf{k}' - \int S(\mathbf{k},\mathbf{k}') f(\mathrm{t},\mathbf{k})\,\big(1-f(\mathrm{t},\mathbf{k}')\big)\,d\mathbf{k}'\,. \tag{7}$$

We take a Fermi-Dirac distribution, as initial condition,

$$f(0,\mathbf{k}) = \frac{1}{1+\exp\left(\dfrac{\varepsilon(\mathbf{k})-\mu}{k_B\,T}\right)},$$

where $T = 300\,\mathrm{K}$, and μ is the chemical potential, that is determined by choosing the initial charge density

$$\rho(0) = \frac{2}{(2\,\pi)^2}\int f(0,\mathbf{k})\,d\mathbf{k}\,. \tag{8}$$

Equation (7) is discretized by adopting a discontinuous Galerkin scheme. We choose a bounded domain $\Omega \subset \mathbb{R}^2$ such that $f(\mathrm{t},\mathbf{k}) \approx 0$ for every $\mathbf{k} \notin \Omega$ and $\mathrm{t} > 0$, and we introduce a finite decomposition $\{C_\alpha\}$ of Ω, with C_α appropriate open set, such that

$$C_\alpha \cap C_\beta = \emptyset \quad \text{if } \alpha \neq \beta, \text{ and } \quad \bigcup_{\alpha=1}^{N} \overline{C_\alpha} = \Omega\,.$$

We assume that the distribution function is constant in each cell C_α. If we denote by $\chi_\alpha(\mathbf{k})$ the characteristic function over the cell C_α, then the approximation of the distribution function f is given by

$$f(\mathrm{t},\mathbf{k}) \approx f^\alpha(\mathrm{t}) \quad \forall\,\mathbf{k} \in C_\alpha \iff f(\mathrm{t},\mathbf{k}) \approx \sum_{\alpha=1}^{N} f^\alpha(\mathrm{t})\,\chi_\alpha(\mathbf{k}) \quad \forall\,\mathbf{k} \in \bigcup_{\alpha=1}^{N} C_\alpha\,.$$

This assumption replaces the unknown f, which depends on the two variables t and $\mathbf{k}$, in a set of N unknowns f^α, which depend only on time t. In order to obtain a set of N equations for the new unknowns f^α, we integrate Eq. (7) with respect to $\mathbf{k}$ over every cell C_α and replace f with its approximation. The derivative of f with respect to the time is treated easily. We have

$$\int_{C_\alpha} \frac{\partial f(\mathrm{t}, \mathbf{k})}{\partial t}\, d\mathbf{k} \approx M_\alpha \frac{df^\alpha}{dt}$$

where M_α is the measure of the cell C_α. It is clear that the numerical method yields a system of ordinary differential equations. This is achieved by discretizing the collision operator and the drift term.

2.1 Discretization of the Collision Operator

Since, for each $\mathbf{k} \in C_\alpha$, we have

$$\begin{aligned}
&\int S(\mathbf{k}', \mathbf{k}) f(\mathrm{t}, \mathbf{k}')\,(1 - f(\mathrm{t}, \mathbf{k}))\, d\mathbf{k}' - \int S(\mathbf{k}, \mathbf{k}') f(\mathrm{t}, \mathbf{k})\left(1 - f(\mathrm{t}, \mathbf{k}')\right) d\mathbf{k}' \\
&\approx \sum_{\beta=1}^{N} \left[\int_{C_\beta} S(\mathbf{k}', \mathbf{k}) f^\beta(\mathrm{t})\,(1 - f^\alpha(\mathrm{t}))\, d\mathbf{k}' - \int_{C_\beta} S(\mathbf{k}, \mathbf{k}') f^\alpha(\mathrm{t})\left(1 - f^\beta(\mathrm{t})\right) d\mathbf{k}' \right] \\
&= \sum_{\beta=1}^{N} \left[f^\beta(\mathrm{t})\,(1 - f^\alpha(\mathrm{t})) \int_{C_\beta} S(\mathbf{k}', \mathbf{k})\, d\mathbf{k}' - f^\alpha(\mathrm{t})\left(1 - f^\beta(\mathrm{t})\right) \int_{C_\beta} S(\mathbf{k}, \mathbf{k}')\, d\mathbf{k}' \right].
\end{aligned}$$

Now, if we define

$$A^{\alpha,\beta} = \int_{C_\alpha} \left[\int_{C_\beta} S(\mathbf{k}, \mathbf{k}')\, d\mathbf{k}' \right] d\mathbf{k}\,, \tag{9}$$

then we obtain

$$\begin{aligned}
&\int_{C_\alpha} \left[\int S(\mathbf{k}', \mathbf{k}) f(\mathrm{t}, \mathbf{k}')\,(1 - f(\mathrm{t}, \mathbf{k}))\, d\mathbf{k}' - \int S(\mathbf{k}, \mathbf{k}') f(\mathrm{t}, \mathbf{k})\left(1 - f(\mathrm{t}, \mathbf{k}')\right) d\mathbf{k}' \right] d\mathbf{k} \\
&\approx \sum_{\beta=1}^{N} \left[A^{\beta,\alpha}\,(1 - f^\alpha(\mathrm{t})) f^\beta(\mathrm{t}) - A^{\alpha,\beta} f^\alpha(\mathrm{t})\left(1 - f^\beta(\mathrm{t})\right) \right].
\end{aligned}$$

So, the integral collision operator is replaced by quadratic polynomials. We note that the numerical coefficients $A^{\alpha,\beta}$ depend only on the scattering terms and the domain decomposition.

2.2 Discretizaton of the Force Term

We must approximate the term

$$-\frac{e}{\hbar}\,\mathbf{E}\cdot\int_{C_\alpha}\nabla_{\mathbf{k}}f(\mathrm{t},\mathbf{k})\,d\mathbf{k} = -\frac{e}{\hbar}\,\mathbf{E}\cdot\int_{\partial C_\alpha} f(t,\mathbf{k})\,\mathbf{n}\,d\sigma$$

where $\mathbf{n}$ is the normal to the boundary ∂C_α of the cell C_α. Since, due to the Galerkin method, the approximation of f is not defined on the boundary of the cells, we must introduce a *numerical flux*, that furnishes reasonable values of f on every ∂C_α, depending on the values of the approximation of f in the nearest neighborhood of the cell C_α and on the sign of $\mathbf{E}\cdot\mathbf{n}$. In Fig. 1 we show a simple picture of the cells that can be involved to find the numerical flux. The simplest numerical flux is given by the *upwind rule*, that use only four nearest adjacent cells.

3 Numerical Simulations

We consider a circle as domain Ω. We used the same physical parameters of [3]. The charge density is taken equal to $10^{12}\,\mathrm{cm}^{-2}$. A TVD third Runge-Kutta scheme is used to solve the resulting ODE system. The numerical scheme is very similar to [11]. We remark that the numerical scheme guarantees the mass conservation. We solve Eq. (7) for different value of the applied electric field. In Fig. 2 we show the macroscopic velocity and energy, defined by

$$\frac{2}{(2\,\pi)^2\,\rho(0)}\int f(t,\mathbf{k})\,v_F\,\frac{\mathbf{k}}{|\mathbf{k}|}\,d\mathbf{k}\,,\qquad \frac{2}{(2\,\pi)^2\,\rho(0)}\int f(t,\mathbf{k})\,\varepsilon(\mathbf{k})\,d\mathbf{k}\,.$$

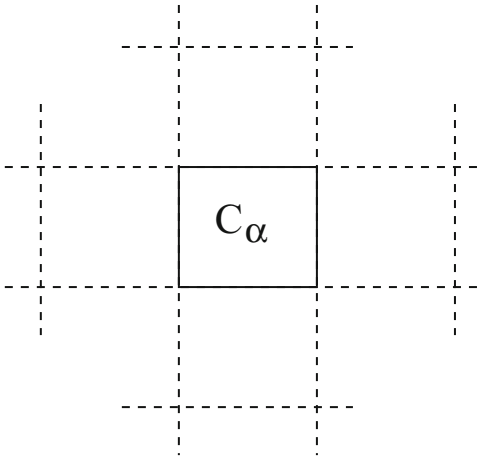

Fig. 1 Cells employed for the numerical flux in the case of a simple rectangular grid

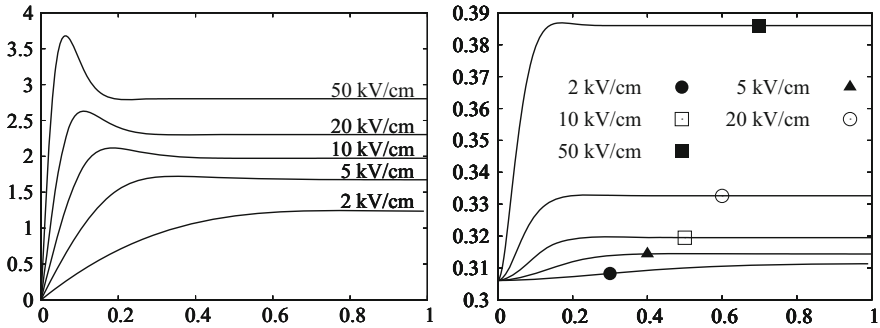

Fig. 2 *Left figure*: the mean velocity in 10^7 cm/s versus time (in ps). *Right figure*: the mean energy in eV versus time (in ps)

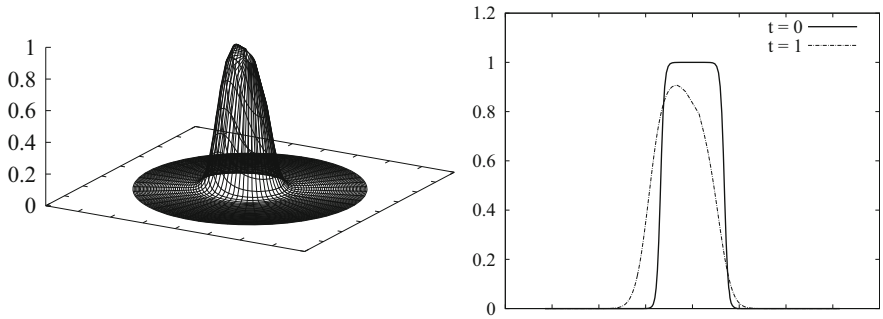

Fig. 3 *Left figure*: The distribution function (electric field equal to 50 kV/cm) at 1 ps. *Right figure*: the section at $k_y = 0$ of the distribution function (electric field equal to 50 kV/cm) at the initial time and at 1 ps

We note that the asymptotic mean velocity and energy increase by increasing the applied voltage. In Fig. 3 we show the distribution function f for the highest electric field.

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