# An Electro-Thermal Hydrodynamical Model for Charge Transport in Graphene

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**Abstract** A hydrodynamical model for the charge and the heat transport in graphene is presented. The state variables are moments of the electron, hole and phonon distribution functions, and their evolution equations are derived from the respective Boltzmann equations by integration. The closure of the system is obtained by means of the maximum entropy principle and all the main scattering mechanisms are taken into account. Numerical simulations are presented in the case of a suspended graphene monolayer.

**Keywords** Charge transport • Electro-thermal hydrodynamical model • Maximum entropy principle

# 1 Introduction

Graphene is among the most promising materials for future applications in nanoelectronics devices. It is two dimensional and consists of a single layer of carbon atoms arranged into a honeycomb hexagonal lattice. Graphene has very good mechanical properties and is an excellent heat and electricity conductor. In order to formulate comprehensive transport models it is necessary to take into account the electronic and phonon bandstructure and the most relevant scattering mechanisms

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between electrons and phonons. The case of a suspended sheet of graphene is considered here.

#### 2 Kinetic Description

Electrons which contribute to the charge transport in graphene are those in the conduction and valence band, and it is preferable to treat the latter as holes for insuring integrability of the distribution function. Electrons and holes mostly populate the states near to the *K* and *K'* Dirac points situated at the boundary of the first hexagonal Brillouin zone, the respective neighborhoods being called *K* and *K'* valleys. In these valleys, the energies  $\epsilon_i$ , i = e, h, (*e* and *h* respectively stay for electrons and holes) are, with a good approximation, linear in the wave vector  $\mathbf{k}$ :  $\epsilon_i = \hbar v_F |\mathbf{k}|$ ,  $\mathbf{k} \in \mathbb{R}^2$ ,  $i = e, h, \hbar$  being the reduced Planck constant, and  $v_F$  the Fermi velocity. *K* and *K'* valleys will be treated as equivalent.

A semiclassical kinetic description of the charge transport in graphene is based on the two Boltzmann equations for electrons and holes (approaches which make use of the Wigner transport equations are also present in the literature, for example, see [1])

$$\frac{\partial f_i}{\partial t} + \mathbf{v}_i \cdot \nabla_{\mathbf{k}} f_i + \frac{\mathbf{e}_i}{\hbar} \mathbf{E} \cdot \nabla_{\mathbf{k}} f_i = \mathscr{C}_i, \quad i = e, h,$$
(1)

where  $f_i(\mathbf{r}, \mathbf{k}, t)$ , i = e, h, represent the state occupation numbers of electrons and holes at position  $\mathbf{r}$ , time t and with wave-vector  $\mathbf{k}$ .  $\nabla_{\mathbf{r}}$  and  $\nabla_{\mathbf{k}}$  are the gradients with respect to the position and the wave vector respectively,  $\mathbf{e}_i$ , i = e, h, are the particle charges (negative for electrons and positive for holes), and  $\mathbf{E}$  is the electric field obtained by the Poisson equation, which must be coupled with the above system. The group velocity  $\mathbf{v}$  is related to the band energy by  $\mathbf{v} = \frac{1}{\hbar} \nabla_{\mathbf{k}} \varepsilon_i = v_F \frac{\mathbf{k}}{|\mathbf{k}|}$ .  $\mathscr{C}_i$ , i = e, h, are the scattering operators representing both the intra and interband interactions of electrons and holes with acoustic and optical phonons. Its complete expression is rather involved, here, for simplicity, we report only the generic contribution relative to the intra-conduction band scattering and refer the interested readers to [2, 3]

$$\mathscr{C}_{e}(\mathbf{k}) = \frac{1}{(2\pi)^{2}} \int_{\mathbb{R}^{2}} \left[ \underbrace{w_{ee}(\mathbf{k}', \mathbf{k}) f_{e}(\mathbf{k}') (1 - f_{e}(\mathbf{k}))}_{gain} - \underbrace{w_{ee}(\mathbf{k}, \mathbf{k}') f_{e}(\mathbf{k}) (1 - f_{e}(\mathbf{k}'))}_{loss} \right] d\mathbf{k}',$$

where  $w_{ee}(\mathbf{k}', \mathbf{k})$  is the transition rate from the state  $\mathbf{k}$  to the state  $\mathbf{k}'$ . In this case, the detailed balance principle implies  $w_{ee}(\mathbf{k}, \mathbf{k}') = e^{(\varepsilon - \varepsilon')/k_B T} w_{ee}(\mathbf{k}', \mathbf{k})$ , with  $k_B$  the Boltzmann constant and T the lattice temperature.

We consider interactions with acoustic phonons, longitudinal optical phonons ( $\Gamma$ -LO), transversal optical phonons ( $\Gamma$ -TO), and *K*-phonons.

In the elastic approximation, the production term relative to acoustic phonon (intraband) transitions simplifies into

$$\mathscr{C}_{i}(\mathbf{k}) = \frac{1}{(2\pi)^{2}} \int_{\mathbb{R}^{2}} A^{(ac)}(1 + \cos \theta'') \delta(\varepsilon_{i}' - \varepsilon_{i}) \left( f_{i}(\mathbf{k}') - f_{i}(\mathbf{k}) \right) d\mathbf{k}'.$$

where  $A^{(ac)}$  can be found in [4–6] and  $\theta''$  is the angle between **k** and **k**'.

For the optical and the *K*-phonons, in the Einstein approximation ( $\hbar \omega = \cos t$ , with  $\omega$  phonon frequency), one has

$$w_{ee}^{s}(\mathbf{k}',\mathbf{k}) = s_{ee}^{s}(\mathbf{k}',\mathbf{k}) \left[ \underbrace{\left( g_{s}^{-}+1 \right) \delta\left( \varepsilon_{e} - \varepsilon_{e}' + \hbar \omega_{s} \right)}_{emission} + \underbrace{g_{s}^{+} \delta\left( \varepsilon_{e} - \varepsilon_{e}' - \hbar \omega_{s} \right)}_{absorption} \right],$$
  
$$s = LO, TO, K,$$

with  $s_{ee}^{K}(\mathbf{k}', \mathbf{k}) = A_{K}D_{K}^{2}(1 - \cos\theta'')$  for the *K*-phonons and  $s_{ee}^{\Gamma}(\mathbf{k}', \mathbf{k}) = A_{\Gamma}D_{\Gamma}^{2}(1 \mp \cos(\theta + \theta'))$  respectively for the *LO* and *TO* phonons.  $A^{K}$  and  $A^{\Gamma}$  can be found in [5, 6], and  $\theta$  and  $\theta'$  respectively denote the angle between  $\mathbf{k}$  and  $\mathbf{k}' - \mathbf{k}$  and that between  $\mathbf{k}'$  and  $\mathbf{k}' - \mathbf{k}$ .

If phonons are considered as a thermal bath at the constant temperature  $T_L$ 

$$g_s^{\pm} \approx \left[ e^{\hbar \omega_s / k_B T_L} - 1 \right]^{-1}$$
, equilibrium Bose-Einstein,

otherwise  $g_s^{\pm} = g_s(\mathbf{r}, t, \mathbf{q}^{\pm})$ , with the phonon wave vector given by  $\mathbf{q}^{\pm} = \pm (\mathbf{k}' - \mathbf{k})$ , in agreement with the momentum conservation.

Moreover, if we consider the phonon dynamics, the evolution of the phonon occupation number is governed by the following Boltzmann equations

$$\begin{split} \frac{\partial g_s}{\partial t} &+ \underbrace{\nabla_{\mathbf{q}} \omega_s(\mathbf{q})}_{\approx 0} \cdot \nabla_{\mathbf{r}} g_s = \mathscr{C}_s, \quad s = LO, TO, K, \\ \frac{\partial g_{ac}}{\partial t} &+ \nabla_{\mathbf{q}} \omega_{ac}(\mathbf{q}) \cdot \nabla_{\mathbf{r}} g_{ac} = \mathscr{C}_{ac}, \\ \mathscr{C}_s &= -\frac{\left(g_s - g_s^0\right)}{\tau_{OA}} + \sum_{ij} \mathscr{C}_s^{ij}, \ i, j = e, h, \ s = LO, TO, K, \\ \mathscr{C}_{ac} &= -\frac{3}{\tau_{OA}} \left(g_{ac} - g_{ac}^0\right) + \sum_i \mathscr{C}_{ac}^i, \quad i = e, h, \end{split}$$

where  $\tau_{OA}$  is the relaxation time for the decay of an optical phonon into two acoustic phonons, and  $g_s^0$ , s = LO, TO, K,  $g_{ac}^0$  are the equilibrium occupation number of the optical and acoustic phonons corresponding to the temperature they would have if

they were at the local equilibrium relative to their total average energy [7]. In the acoustic phonon scattering, normal and umpklapp types of intra-mode interactions as well as interactions with defects/impurities should also be considered.

Direct simulations based on the above-written semiclassical kinetic equations have been performed by MC methods, see e.g. [5], or with suitable numerical schemes [6], but they, even if very accurate, are too heavy from a computational point of view. Therefore models based on integrated quantities are preferable for computer aided design (CAD) purposes in view of a possible use of graphene in electron devices like MOSFETs or DG-MOSFETs.

#### **3** Carrier Moment Equations

Macroscopic quantities can be defined as moments of the distribution functions with respect to some suitable weight functions  $\psi(\mathbf{k})$ , assuming a sufficient regularity for the existence of the involved integrals. In particular for electrons and holes we propose a set of moment equations consisting of the balance equations of the quantities (i = e, h)

average density 
$$\rho_i = \frac{4}{(2\pi)^2} \int_{\mathbb{R}^2} f_i(\mathbf{r}, \mathbf{k}, t) d\mathbf{k}$$
,  
average velocity  $\rho_i \mathbf{V}_i = \frac{4}{(2\pi)^2} \int_{\mathbb{R}^2} f_i(\mathbf{r}, \mathbf{k}, t) \mathbf{v} d\mathbf{k}$ ,  
average energy  $\rho_i W_i = \frac{4}{(2\pi)^2} \int_{\mathbb{R}^2} f_i(\mathbf{r}, \mathbf{k}, t) \varepsilon d\mathbf{k}$ ,  
average energy-flux  $\rho_i \mathbf{S}_i = \frac{4}{(2\pi)^2} \int_{\mathbb{R}^2} f_i(\mathbf{r}, \mathbf{k}, t) \varepsilon \mathbf{v} d\mathbf{k}$ ,

where the factor 4 arises from taking into account both the spin states and the two equivalent valleys.

By integrating the Boltzmann equations with respect to  $\mathbf{k}$ , one has the following balance equations for the above-defined macroscopic quantities

$$\begin{aligned} &\frac{\partial}{\partial t}\rho_{i} + \nabla_{\mathbf{r}}\cdot(\rho_{i} \ \mathbf{V}_{i}) = \rho_{i} C_{i}, \\ &\frac{\partial}{\partial t}\left(\rho_{i} \ \mathbf{V}_{i}\right) + \nabla_{\mathbf{r}}\cdot\left(\rho_{i} \ \mathbf{F}_{i}^{(0)}\right) - \mathbf{e}_{i} \rho_{i} \mathbf{G}_{i}^{(0)} \cdot \mathbf{E} = \rho_{i} C_{\mathbf{V}_{i}}, \\ &\frac{\partial}{\partial t}\left(\rho_{i} W_{i}\right) + \nabla_{\mathbf{r}}\cdot(\rho_{i} \ \mathbf{S}_{i}) - \mathbf{e}_{i} \rho_{i} \mathbf{E} \cdot \mathbf{V}_{i} = \rho_{i} C_{W_{i}}, \\ &\frac{\partial}{\partial t}\left(\rho_{i} \ \mathbf{S}_{i}\right) + \nabla_{\mathbf{r}}\cdot\left(\rho_{i} \ \mathbf{F}_{i}^{(1)}\right) - \mathbf{e}_{i} \rho_{i} \mathbf{G}_{i}^{(1)} \cdot \mathbf{E} = \rho_{i} C_{\mathbf{S}_{i}}, \end{aligned}$$

where the G's and F's are extra-fluxes and the terms at the right hand sides are productions [3].

### 4 The Phonon Moment System

Similarly for each type of phonons we have

$$\frac{\partial}{\partial t}W_p + \nabla_{\mathbf{r}} \cdot \mathbf{Q}_p = C_{W_p}, \text{ energy balance equation,}$$
$$\frac{\partial}{\partial t}\mathbf{Q}_p + \nabla_{\mathbf{r}} \cdot \mathbf{T}_p = C_{\mathbf{Q}_p}, \text{ energy-flux balance equation.}$$

where for each phonon mode

$$W_p = \int_{\mathscr{B}} \hbar \omega_p g_p \, d\mathbf{q}, \quad \text{average energy,}$$
$$\mathbf{Q}_p = \int_{\mathscr{B}} \hbar \omega_p \mathbf{v}_p g_p \, d\mathbf{q}, \quad \text{average energy-flux}$$

 $\mathscr{B}$  is the hexagonal Brillouin zone and p = LO, TO, K, ac, the T's are extra-fluxes, and the terms at the right hand sides are productions [3]. More general moment systems can be considered, that we consider here is the minimal one for a reasonable description of the thermo-electrical effects.

# 5 The Closure Problem

The extra fluxes and the production terms are additional unknown quantities. For them constitutive relations in terms of the fundamental variables are needed in order to get a closed system of balance equations. A well theoretically founded way to get the desired closure relations is to resort to the Maximum Entropy Principle (MEP) [8], according to which the electron, hole and phonon distribution functions can be estimated by the distributions  $f_{e,MEP}$ ,  $f_{h,MEP}$ ,  $g_{p,MEP}$  which solve the following problem:

$$(f_{e,MEP}, f_{h,MEP}, g_{P,MEP}) = \max_{f_e, f_h, g_p \in L^1(\mathbb{R}^2)} S[f_e, f_h, g_p]$$

under the constraints

$$\begin{pmatrix} \rho_i \\ \rho_i W_i \end{pmatrix} = \frac{2}{(2\pi)^2} \int_{\mathbb{R}^2} \begin{pmatrix} 1 \\ \varepsilon \end{pmatrix} f_i(\mathbf{r}, \mathbf{k}, t) \, d\mathbf{k},$$
$$\begin{pmatrix} \rho_i \mathbf{V}_i \\ \rho_i \mathbf{S}_i \end{pmatrix} = \frac{2}{(2\pi)^2} \int_{\mathbb{R}^2} f_i(\mathbf{r}, \mathbf{k}, t) \begin{pmatrix} \mathbf{v} \\ \varepsilon \mathbf{v} \end{pmatrix} \, d\mathbf{k},$$
$$W_p = \int_{\mathbb{R}^2} \hbar \omega_p g_p \, d\mathbf{q}, \quad \mathbf{Q}_p = \int_{\mathbb{R}^2} \hbar \omega_p \mathbf{v}_p g_p \, d\mathbf{q},$$

where  $S[f_e, f_h, g_p]$  is the total entropy of the system given by

$$-k_{B}\left\{\frac{4}{(2\pi)^{2}}\int_{\mathbb{R}^{2}}\left[f^{e}\ln f^{e}+(1-f^{e})\ln(1-f^{e})\right]d\mathbf{k}+\frac{4}{(2\pi)^{2}}\int_{\mathbb{R}^{2}}\left[f^{h}\ln f^{h}+(1-f^{h})\ln(1-f^{h})\right]d\mathbf{k}+\sum_{p}y^{p}\int_{\mathscr{B}}\left(1+\frac{g^{p}}{y^{p}}\right)\ln\left(1+\frac{g^{p}}{y^{p}}\right)\right]d\mathbf{q}\right\},$$

 $y^p$  being the phonon densities of states and  $L^1(\mathbb{R}^2)$  the usual Banach space.

By solving the above maximization problem we get

$$f_i = \frac{1}{1 + \exp\left(\lambda_i + \lambda_{W_i}\varepsilon_i + \mathbf{v}_i \cdot (\lambda_{\mathbf{v}_i} + \varepsilon_i\lambda_{\mathbf{S}_i})\right)}, \ g_p = \frac{1}{\exp\left(\lambda_{W_p}\varepsilon_p + \varepsilon_p \mathbf{v}_p \cdot \lambda_{\mathbf{Q}_p}\right) - 1}.$$

As in [9–12] we linearize the distributions around their anisotropic part, obtaining

$$f_{i} \approx \frac{1}{e^{\lambda_{i} + \lambda_{W_{i}}\varepsilon_{i}} + 1} \left[ 1 - \frac{e^{\lambda_{i} + \lambda_{W_{i}}\varepsilon_{i}}}{e^{\lambda_{i} + \lambda_{W_{i}}\varepsilon_{i}} - 1} \mathbf{v}_{i} \cdot (\lambda_{\mathbf{v}_{i}} + \varepsilon_{i}\lambda_{\mathbf{S}_{i}}) \right], \ i = e, h,$$

$$g_{p} \approx \frac{1}{e^{\lambda_{W_{p}}\varepsilon_{p}} - 1} \left[ 1 - \frac{e^{\lambda_{W_{p}}\varepsilon_{p}}}{e^{\lambda_{W_{p}}\varepsilon_{p}} - 1} \epsilon_{p} \mathbf{v}_{p} \cdot \lambda_{\mathbf{Q}_{p}} \right], \ p = LO, TO, K, ac,$$

where the  $\lambda$ 's are Lagrange multipliers which have to be expressed as functions of the state variables by taking into account the constraints.

After that, these distributions are inserted into the kinetic definitions of the additional variables, so closing the system of the balance equations. For example, for the optical phonons we obtain  $C_{W_s} = \sum_{ij} C_{W_s}^{ij} + C_{W_s}^{ac}$ , where the sum is for

 $(i,j) \in \{(e,h), (e,e), (h,h)\},$  and

$$C_{W_{s}}^{eh} = \frac{2D_{s}^{2}}{2\pi^{2}\rho\hbar^{3}v_{F}^{4}} \int_{0}^{\epsilon_{s}} \varepsilon(\epsilon_{s}-\varepsilon)\chi_{s}^{eh} \left(\frac{\epsilon_{s}-\varepsilon}{\varepsilon}\right) g^{0}(\epsilon_{s})$$

$$\times \mathscr{F}_{FD}^{e}(\varepsilon)\mathscr{F}_{FD}^{h}(\epsilon_{s}-\varepsilon) \left[ e^{\epsilon_{s}\lambda_{W_{s}}} - e^{\lambda_{e}+\lambda_{h}+\lambda_{W_{e}}\varepsilon} e^{\lambda_{W_{h}}(\epsilon_{s}-\varepsilon)} \right] d\varepsilon,$$

$$C_{W_{s}}^{ee} = \frac{1}{\pi^{2}\rho\hbar^{3}v_{F}^{4}} D_{s}^{2} \int_{0}^{\infty} \varepsilon(\varepsilon+\epsilon_{s})\chi_{s}^{ee} \left(\frac{\epsilon_{s}+\varepsilon}{\varepsilon}\right) g^{0}(\epsilon_{s})$$

$$\times \mathscr{F}_{FD}^{e}(\varepsilon)\mathscr{F}_{FD}^{e}(\varepsilon+\epsilon_{s}) \left[ e^{\epsilon_{s}\lambda_{W_{s}}+\lambda_{e}+\lambda_{W_{e}}\varepsilon} - e^{\lambda_{e}+\lambda_{W_{e}}\varepsilon} e^{\lambda_{W_{e}}\epsilon_{s}} \right] d\varepsilon.$$

$$C_{W_{s}}^{ae} = \frac{A\epsilon_{s}}{\tau_{OA}} \left[ g^{0} \left(\epsilon_{s}, \frac{1}{k_{B}T_{OA}}\right) - g^{0} \left(\epsilon_{s}, \lambda_{W_{s}}\right) \right],$$

 $\rho$  being the area density of graphene, *A* the area of the first Brillouin zone,  $\mathscr{F}_{FD}$  the equilibrium Fermi-Dirac occupation number,  $T_{OA}$  the phonon local equilibrium temperature,  $\epsilon_s$  the optical phonon energy, while the functions  $\chi_s^{ij}$ , i, j = e, h, s = LO, TO, K, and the relaxation time  $\tau_{OA}$  can be found in [3]. Neglecting the acoustic phonon dynamics, the simplest way to study the effect of lattice heating is to use a temperature *T* which empirically depends on the total current, that is  $T = T_L + \gamma \frac{IU}{L}$ , where *I* is the total current, *U* the applied voltage bias, *L* the device length, and  $\gamma$  can be found in [6].

## 6 Numerical Simulations

In the literature there are several values for the coupling constants entering into the collision terms. For example for the acoustic deformation potential one can find values ranging from 2.6 to 29 eV. Similar degree of uncertainty is found for the optical and K phonon coupling constants as well. We have performed numerical simulations of a suspended graphene monolayer by considering the parameters used in [13], see Figs. 1 and 2.

For moderate applied fields the asymptotic value of the electron velocity increases with the applied field, while for high electric fields the velocity decreases (negative differential conductivity) but there is no velocity saturation. The results are consistent with the Monte Carlo simulations presented in [14].

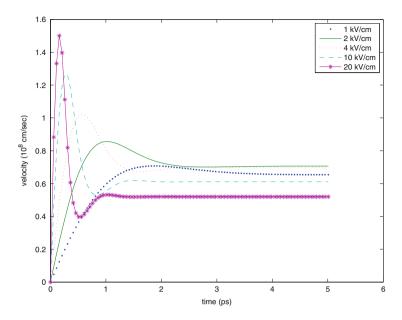
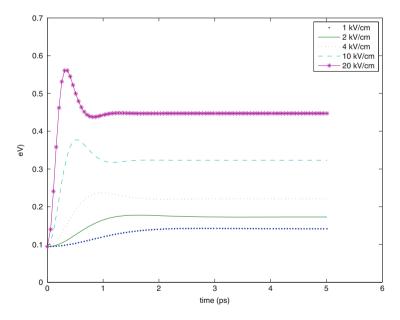


Fig. 1 Average velocity for the electric fields E = 1 kV/cm, E = 2 kV/cm, E = 4 kV/cm, E = 10 kV/cm, E = 20 kV/cm by using the same values of the scattering parameters as in [13], by considering a constant lattice temperature of 300 K and a carrier density equal to  $10^{12} \text{ cm}^{-2}$ 



**Fig. 2** Average energy for the electric fields E = 1 kV/cm, E = 2 kV/cm, E = 4 kV/cm, E = 10 kV/cm, E = 20 kV/cm by using the same values of the scattering parameters as in [13], by considering a constant lattice temperature of 300 K and a carrier density equal to  $10^{12} \text{ cm}^{-2}$ 

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