A comprehensive hydrodynamical model for charge transport in graphene nano-ribbons

G. Mascali, and V. Romano*
Dipartimento di Matematica ed Informatica, Università della Calabria, and INFN-Gruppo c. Cosenza,
87036 Cosenza, Italia, email: giovanni.mascali@unical.it
*Dipartimento di Matematica ed Informatica, Università di Catania, 95125 Catania, Italia
e-mail: romano@dmi.unict.it

INTRODUCTION

Graphene is a very promising material for future applications in nano electronics devices. It is a two dimensional material consisting 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 very high quality graphene very few defects are present, which makes the contribution of phonons to resistivity at room temperature very important and motivates the formulation of comprehensive transport models taking into account electrons in the conduction and valence bands, as well as phonons. The case of a suspended sheet of graphene will be considered.

I. THE MACROSCOPIC MODEL

We treat the electrons in the valence band as holes in order to overcome some integrability problems for the moments of the distribution function and have a more symmetric description between the valence and the conduction band [1]. The most of electrons are in the valleys around the vertices of the Brillouin zone, called Dirac points or K and K' points [2]. We will treat the three K-valley and the three K'-valleys as equivalent to a single valley. With a very good approximation a linear dispersion relation can be used both for electron and hole energies

$$\mathcal{E}_i = \hbar v_F \left|\mathbf{k}\right|,\ i = e, h,$$

$\hbar$ being the reduced Planck constant, v_F the Fermi velocity, and $\mathbf{k}$ the wave vector. We describe the physical state of electrons and holes by using the moments of their respective distribution functions, f_i, $i = e, h$, corresponding to the microscopic weight functions $\{1, \mathbf{v}_i(\mathbf{k}), \mathcal{E}_i, \mathcal{E}_i\mathbf{v}_i(\mathbf{k})\}$. These moments are

$$n_i,\ \mathbf{V}_i,\ W_i,\ \mathbf{S}_i,\ i = e, h,$$

which respectively represent the number densities, average velocities, energies and flux energies of electrons and holes. Different choices of the fundamental macroscopic variables can be found in the literature, see for example [3]. Direct simulations based on semiclassical kinetic equations have been performed in [4] but they, even if very accurate, are still too heavy from a computational point of view and therefore models based on integrated quantities, as those proposed above, are preferable for CAD purposes.

As regards phonons, three types of optical phonons and one type of acoustic phonons are considered, those which significantly contribute to the electron scattering in graphene. Among these, the longitudinal optical (Γ-LO phonons) and transversal optical phonons (Γ-TO phonons) have wave vectors close to the Γ-point in the Brillouin zone, and energies $\hbar\omega_{LO} = \hbar\omega_{TO} = 196\,\text{meV}$, while the zone boundary phonons (K phonons), with $\hbar\omega_K = 161\,\text{meV}$, are close to the K-point. Their dispersions are very flat, therefore, following the Einstein approximation, the above energies are used for all phonon wave vectors $\mathbf{q}$ sufficiently close to the Γ and the K-point respectively. The state of the optical phonons is described by using the moments of their respective distribution functions g_η, $\eta = LO, TO, K$, corresponding to the weight functions $\epsilon_\eta, \hbar\mathbf{q}$, that is

$$W_\eta,\ \mathbf{P}_\eta,\ \eta = LO, TO, K,$$

which respectively represent the energy and the momentum densities of the three families of optical phonons.

The relevant acoustic phonons (ac-phonons) are of longitudinal type and have wave vectors close to the Γ-point. Their state is described by using only their temperature T as in [4].

The evolution equations for the electron, hole, and longitudinal optical state variables are obtained by taking the moments of the respectively Boltzmann equations.

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All the scattering mechanisms described in [4] are taken into account, that is the intraband and interband scatterings of electrons with optical phonons, the quasi-elastic intraband scattering of electrons with acoustic phonons, and the decay of an optical phonon into two acoustic phonons. In the evolution equations besides the state variables, extra variables appear, which are fluxes and production terms. In the following we write only the equations for the optical phonon variables, those for electrons and holes can be found in [1]

$$\begin{aligned}\frac{\partial W_\eta}{\partial t} &= C_{W_\eta},\\ \frac{\partial \mathbf{P}_\eta}{\partial t} &= C_{\mathbf{P}_\eta},\ \eta = LO, TO, K,\end{aligned}$$

where C_{W_η} and $C_{\mathbf{P}_\eta}$ are the energy and momentum productions due to scatterings with electrons and holes and to the decay of optical phonons into acoustic ones [5]. The closure of the evolution equations is obtained by using, in the expressions of the extra variables as integrals of the distribution functions, the following almost isotropic maximum entropy distribution functions [1], [5], [6], [7]

$$\begin{aligned}f_i &= \frac{y_i}{e^{\lambda_i+\lambda_{W_i}\mathcal{E}_i}-1}\left[1-\frac{e^{\lambda_i+\lambda_{W_i}\mathcal{E}_i}}{e^{\lambda_i+\lambda_{W_i}\mathcal{E}_i}-1}\,\mathbf{v}_i\cdot(\lambda_{\mathbf{V}_i}\right.\\ &\quad \left.+\mathcal{E}_i\lambda_{\mathbf{S}_i})\right],\ y_i=\frac{2}{(2\pi)^2},\ i=e,h,\\ g_\eta &= \frac{y_\eta}{e^{\lambda_{W_\eta}\epsilon_\eta}-1}\left[1-\frac{e^{\lambda_{W_\eta}\epsilon_\eta}}{e^{\lambda_{W_\eta}\epsilon_\eta}-1}\,\hbar\mathbf{q}\cdot\lambda_{\mathbf{P}_\eta}\right],\\ &\quad y_\eta=\frac{1}{(2\pi)^2},\ \eta=LO,TO,K,\end{aligned}$$

where the λ's are Lagrange multipliers which have to be expressed as functions of the state variables by taking into account that these latter are moments of the distribution functions. So doing, for example, we obtain

$$C_{W_\eta} = \sum_{ij} C^{ij}_{W_\eta} + C^{ac}_{W_\eta},$$

where the sum is for $(i,j)\in\{(e,h),(e,e),(h,h)\}$, and

$$\begin{aligned}C^{eh}_{W_\eta} &= \frac{1}{2\pi^2\rho\hbar^3 v_F^4}D_\eta^2\int_0^{2\pi}\int_0^{\epsilon_\eta}\mathcal{E}(\epsilon_\eta-\mathcal{E})\\ &\quad\cdot\chi^{eh}_\eta(\mathcal{E},\phi'')\mathcal{F}_{BE}(\epsilon_\eta)\mathcal{F}^e_{FD}(\mathcal{E})\mathcal{F}^h_{FD}(\epsilon_\eta-\mathcal{E})\\ &\quad\cdot\left[e^{\epsilon_\eta\lambda_{W_\eta}}-e^{\lambda_e+\lambda_h+\lambda_{W_e}\mathcal{E}+\lambda_{W_h}(\epsilon_\eta-\mathcal{E})}\right]d\mathcal{E}d\phi'',\\ C^{ii}_{W_\eta} &= \frac{1}{2\pi^2\rho\hbar^3 v_F^4}D_\eta^2\int_0^{2\pi}\int_0^{\infty}\mathcal{E}(\mathcal{E}+\epsilon_\eta)\\ &\quad\cdot\chi^{ii}_\eta(\mathcal{E},\phi'')\mathcal{F}_{BE}(\epsilon_\eta)\mathcal{F}^i_{FD}(\mathcal{E})\mathcal{F}^i_{FD}(\mathcal{E}+\epsilon_\eta)\\ &\quad\cdot\left[e^{\epsilon_\eta\lambda_{W_\eta}+\lambda_i+\lambda_{W_i}\mathcal{E}}-e^{\lambda_i+\lambda_{W_i}(\mathcal{E}+\epsilon_\eta)}\right]d\mathcal{E}d\phi'',\end{aligned}$$

$$C^{ac}_{W_\eta} = \frac{A}{\tau_n}\left[\mathcal{F}_{BE}\Big(\epsilon_\eta,\frac{1}{K_BT_L}\Big)-\mathcal{F}_{BE}\Big(\epsilon_\eta,\lambda_{W_\eta}\Big)\right],$$

with $i=e,h$, ρ being the area density of graphene, A the area of the Brillouin zone, K_B the Boltzmann constant, $\mathcal{F}_{BE}$ and $\mathcal{F}_{FD}$ the Bose-Einstein and the Fermi-Dirac occupation numbers, T_L is the constant lattice temperature, and the functions χ^{ij}_η, $i,j=e,h$, $\eta=LO,TO,K$, and the relaxation time τ_n can be found in [8]. The temperature T is modeled by means of the formula $T=T_L+\gamma\frac{IU}{L}$, where I is the total current, U the applied voltage bias, L the device length, and γ can be found in [4].

Conclusion

In this work we present a comprehensive macroscopic model for describing the charge transport in graphene nano-ribbons, which takes into account the main scattering mechanisms to which electrons are subject to, and the dynamics of the optical phonons. Simulations are under current investigation.

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