

## HYDRODYNAMICAL MODELS FOR CHARGE TRANSPORT IN GRAPHENE BASED ON THE MAXIMUM ENTROPY PRINCIPLE: THE CASE OF MOMENTS BASED ON ENERGY POWERS

LILIANA LUCA<sup>a</sup> AND VITTORIO ROMANO<sup>a\*</sup>

**ABSTRACT.** Hydrodynamical models for charge transport in graphene can be obtained as moment equations of the semiclassical Boltzmann equation in which the needed closure relations are obtained by resorting to the Maximum Entropy Principle (Jaynes 1957; Müller and Ruggeri 1998; Mascali and Romano 2005; Jou and Lebon 2010). Several choices of the weight functions defining the moments can be made. The aim of this paper is analyzing the case in which the moments are expectation values of powers of the energy and a comparison is performed with the results given by directly solving the transport equation through the method in Romano *et al.* (2015) and Coco *et al.* (2016b). It has been found out that adding new moments, representing further expectation values of powers of energy, with respect to those already considered in Camiola and Romano (2014) does not improve the accuracy of the model.

### 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 new semiconductor material for future applications in nano-electronic (Neto *et al.* 2009; Lichtenberger *et al.* 2011; Barletti 2014; Morandi and Barletti 2014) and optoelectronic devices (Zhao *et al.* 2015).

A physically accurate model for charge transport is given by a semiclassical Boltzmann equation (quantum effects have also been included in the literature, e.g. see Morandi and Schürer (2011) and Barletti (2016)). Usually, the available solutions have been obtained with direct Monte Carlo simulations, e.g. a new Direct Simulation Monte Carlo (DSMC) procedure has been devised in Romano *et al.* (2015), Coco *et al.* (2016b), and Majorana and Romano (2017) 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 Lichtenberger *et al.* (2011) while a Discontinuous Galerkin (DG) method has been used in Romano *et al.* (2015), Coco *et al.* (2016a), and Majorana *et al.* (2016)

---

*This paper is dedicated to the memory of Prof. Gaetano Giaquinta (1945–2016)*

(for algorithms of the Wigner equation see Muscato and Wagner (2016)). However, due to the computational difficulties related to the DSMC or deterministic solutions of the semiclassical Boltzmann equation, in view of applications in future electronic devices, it is desirable to have also macroscopic models for charge transport in graphene like drift-diffusion, energy transport and hydrodynamical models which are more suited for Computer Aided Design (CAD) purposes.

A hydrodynamical model based on the maximum entropy principle (MEP) has been formulated in Camiola and Romano (2014) using a set of field variables which proved to be successful for traditional semiconductors like silicon (Romano 2002; Mascali and Romano 2005; Romano 2007; Rosa and Romano 2008; Rosa *et al.* 2009; Muscato and Stefano 2013; Mascali 2016), gallium arsenide (Mascali and Romano 1997, 2005), and silicon carbide (Alì *et al.* 2012). Here, we try to improve this model by adding, among the moments, the average flux of higher powers of energy. The accuracy of the model is investigated by a comparison, in the case of suspended monolayer graphene, with the direct solution of the semiclassical Boltzmann equation obtained by the DG method proposed in Romano *et al.* (2015) and Coco *et al.* (2016b). It turns out that including the additional moments of the above mentioned type does not lead to any improvement. Therefore, if more accurate solutions are needed at high electric fields, apparently it is necessary to augment the model in Camiola and Romano (2014) with additional moments. The plan of the paper is as follows. In section 2 the main features of the semiclassical transport equation in graphene are recalled and then, in the next section, general considerations regarding hydrodynamical models are presented. In section 4 a new hydrodynamical model is formulated and its mathematical main features are analyzed in section 5. In the last section the validity of the new model is assessed by comparing the expectation values of velocity and energy with those obtained from the direct solutions of the Boltzmann equation, in the case of suspended monolayer graphene, for several values of the Fermi energy and electric field.

## 2. Kinetic description

The atoms in graphene form two interpenetrating triangular Bravais sub-lattices and each unit cell contains two atoms belonging to different sub-lattices (Neto *et al.* 2009). The first Brillouin zone is hexagonal like the Bravais lattice.

In the proximity of the Dirac points  $K$  ( $K'$ ), that are the vertices of the Brillouin zone, if we choose in the  $\mathbf{k}$ -space a reference frame centered in the considered Dirac point, the energy dispersion relation can be approximated by

$$\mathcal{E}(\mathbf{k}) = \pm \hbar v_F |\mathbf{k}|, \quad (1)$$

with  $v_F \simeq 1 \times 10^6$  cm/s the Fermi velocity,  $\hbar$  the reduced Planck's constant and  $\mathbf{k}$  is the wave vector. The upper sign refers to the conduction band while the lower one refers to the valence band. This approximation is used in the present paper and the first Brillouin zone is extended to all  $\mathbb{R}^2$ .

In a semiclassical kinetic setting, the charge transport in graphene is described by two Boltzmann equations, one for electrons in the valence band and one for electrons in the conduction band in each set of equivalent Dirac points ( $K$  or  $K'$ ). In the following, for the sake of simplicity, we will consider only the conduction band but the results can be easily extended in order to include the valence band. Therefore, we will consider a unique

Boltzmann equation

$$\frac{\partial f(\mathbf{r}, \mathbf{k}, t)}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{r}} f(\mathbf{r}, \mathbf{k}, t) - \frac{q}{\hbar} \mathbf{E} \cdot \nabla_{\mathbf{k}} f(\mathbf{r}, \mathbf{k}, t) = \mathcal{C}[f](\mathbf{r}, \mathbf{k}, t) \quad (2)$$

for the distribution  $f(\mathbf{r}, \mathbf{k}, t)$  of electrons in the conduction band (the dependence from the Dirac point is omitted). As a consequence, in the collision term only intraband scatterings will be considered.

$\nabla_{\mathbf{r}}$  and  $\nabla_{\mathbf{k}}$  are the gradients with respect to the position and wave vector respectively,  $q$  is the elementary (positive) charge and  $\mathbf{v}$  is the microscopic velocity which is related to the energy band by  $\mathbf{v}(\mathbf{k}) = \frac{1}{\hbar} \nabla_{\mathbf{k}} \mathcal{E}(\mathbf{k}) = v_F \frac{\mathbf{k}}{k}$ . The electric field  $\mathbf{E}$  is assumed as external and constant.

$\mathcal{C}$  is the collision term representing the interactions of electrons with acoustic (ac) phonons, longitudinal (*LO*) and transversal (*TO*) optical phonons, and *K*-phonons.

The acoustic, *LO* and *TO* phonons are in-plane (with respect to the plane of the lattice) modes. They give rise to electron intravalley transitions, which mostly involve phonons with wave vectors near to the center  $\Gamma$  of the Brillouin zone (for this reason they are also called  $\Gamma$  phonons). The wave vectors  $\mathbf{q}$  of these phonons are close to zero. Therefore, the acoustic phonon energy is negligible, being with good accuracy linear in the wave vector, while for the dispersion relations of *LO* and *TO* phonons the Einstein approximation can be used, according to which  $\hbar\omega \approx \text{const}$ , with  $\omega$  the phonon frequency. The transitions involving *LO* and *TO* phonons can be both intraband and interband.

The *K*-phonons are not a real phonon branch. Their name is due to the fact that their wave vectors are close to the *K* or *K'* point (Lichtenberger *et al.* 2011). They belong to an optical branch and induce intervalley scatterings. An Einstein approximation with a mean phonon energy is used for them.

Interaction of electrons with out of plane phonon modes, the so-called *Z* phonons, or with in-plane phonons having wave vectors far from the  $\Gamma$  or *K* point, is negligible (Borysenko *et al.* 2010), even though these phonons can play some role in the thermal effects. For an accurate description of phonon dispersion relations and thermal conductivity in graphene, we refer the interested reader to Nika and Balandin (2012) and Pop *et al.* (2012).

As said before, the collision term is given by the sum of the contributions of the several types of scatterings. The generic term due to a single scattering from a state  $\mathbf{k}$  in the *A*-band to a state  $\mathbf{k}'$  in the *B*-band reads (omitting the dependence on space and time for simplifying the notation)

$$\begin{aligned} \mathcal{C}[f](\mathbf{r}, \mathbf{k}, t) = & \frac{1}{(2\pi)^2} \sum_{s=ac, LO, TO, K} \int_{\mathbb{R}^2} \left[ w^{(s)}(\mathbf{k}', \mathbf{k}) f(\mathbf{k}') (1 - f(\mathbf{k})) \right. \\ & \left. - w^{(s)}(\mathbf{k}, \mathbf{k}') f(\mathbf{k}) (1 - f(\mathbf{k}')) \right] d^2 \mathbf{k}' \end{aligned} \quad (3)$$

where  $w^{(s)}(\mathbf{k}', \mathbf{k})$  is the transition rate. It is important to remark that, due to the peculiar band structure, in particular the zero energy gap, the Pauli exclusion principle plays a significant role and the use of a linearized collision operator is not physically accurate. For the sake of conciseness, the dependence on the band indices *A* and *B* will be not explicitly indicated unless when necessary. In the case of acoustic phonons, coherently with the previous considerations, one considers the elastic approximation ( $\hbar\omega_{ac} \approx 0$ ). Therefore the

collision is intraband and can be written as

$$\frac{1}{(2\pi)^2} \int_{\mathbb{R}^2} w^{(ac)}(\mathbf{k}', \mathbf{k}) (f^A(\mathbf{k}') - f^A(\mathbf{k})) d^2\mathbf{k}', \quad (4)$$

where  $w^{(ac)}(\mathbf{k}', \mathbf{k}) = A^{(ac)}(1 + \cos \theta'') \delta(\mathcal{E}_A(\mathbf{k}') - \mathcal{E}_A(\mathbf{k}))$  with  $A^{(ac)} = \frac{\pi D_{ac}^2 k_B T_L}{2\sigma \hbar v_{ac}^2}$ . Here  $\theta''$  is the convex angle between  $\mathbf{k}$  and  $\mathbf{k}'$ ,  $D_{ac}^2$  is the acoustic phonon coupling constant,  $v_{ac}$  is the sound speed in graphene,  $\sigma$  is the graphene areal density,  $k_B$  the Boltzmann constant and  $T_L$  the graphene lattice temperature, which will be kept constant.

For a generic optical phonon interaction and a  $K$ -phonon interaction from a state in the band  $A$  to a state in the band  $B$  the transition rate splits as

$$w_{AB}^{(s)}(\mathbf{k}, \mathbf{k}') = w_{AB}^{(s,+)}(\mathbf{k}, \mathbf{k}') + w_{AB}^{(s,-)}(\mathbf{k}, \mathbf{k}'), \quad s = LO, TO, K,$$

where  $w_{AB}^{(s,+)}(\mathbf{k}, \mathbf{k}')$  and  $w_{AB}^{(s,-)}(\mathbf{k}, \mathbf{k}')$  represent emission and absorption processes respectively.

In the case  $s = LO, TO$  one has

$$w^{(s,\pm)}(\mathbf{k}, \mathbf{k}') = A^{(s)} D_{\Gamma}^2 [1 - \eta_s \cos(\theta + \theta')] \left( N_B^s + \frac{1}{2} \pm \frac{1}{2} \right) \delta(\mathcal{E}(\mathbf{k}') - \mathcal{E}(\mathbf{k}) \pm \hbar\omega_s) \quad (5)$$

where  $A^{(s)} = \pi/\sigma\omega_s$ ,  $D_{\Gamma}^2$  is the optical phonon coupling constant and  $N_B^s$  is the Bose-Einstein distribution

$$N_B^s = \frac{1}{e^{\hbar\omega_s/k_B T_L} - 1}$$

with  $\hbar\omega_s$  phonon energy.  $\theta$  and  $\theta'$  are the convex angles between  $\mathbf{k}$  and  $\mathbf{k}' - \mathbf{k}$  and between  $\mathbf{k}'$  and  $\mathbf{k}' - \mathbf{k}$ .  $\eta_s$  is a parameter which takes the following values

$$\eta_s = \begin{cases} 1 & \text{if } s = LO \\ -1 & \text{if } s = TO \end{cases}.$$

In the sequel  $\hbar\omega_{LO}$  and  $\hbar\omega_{TO}$ , accordingly to the data reported in the literature, are considered as equal and its common value will be denoted by  $\hbar\omega_{OP}$ . Therefore, the distributions of  $LO$  and  $TO$  phonons will be the same and will be denoted by  $N_B^{OP}$ .

If  $s = K$  transition rate is given by

$$w^{(K,\pm)}(\mathbf{k}, \mathbf{k}') = A^{(K)} D_K^2 (1 - \cos \theta'') \left( N_B^K + \frac{1}{2} \pm \frac{1}{2} \right) \delta(\mathcal{E}_B(\mathbf{k}') - \mathcal{E}_A(\mathbf{k}) \pm \hbar\omega_K) \quad (6)$$

where  $A^{(K)} = \pi/\sigma\omega_K$  and  $D_K^2$  is the  $K$ -phonon coupling constant.

At equilibrium the distribution of electrons both in the conduction and valence band is given by the Fermi-Dirac distribution

$$f_{FD}(\mathbf{k}) = \frac{1}{1 + \exp\left(\frac{\mathcal{E}(\mathbf{k}) - \varepsilon_F}{k_B T_L}\right)}, \quad (7)$$

with  $\varepsilon_F$  the Fermi energy. The lattice temperature  $T_L$  will be considered constant and equal to 300 K. In pristine graphene  $\varepsilon_F = 0$  but applying a gate voltage it is possible to modify the value of  $\varepsilon_F$  creating a kind of doping like in conventional semiconductors. If  $\varepsilon_F$  is positive and high enough, one has a sort of  $n$ -doping and the only relevant contribution to the current

is due to the electrons in the conduction band. This is the situation that will be considered in the rest of the article. Analogously, if  $\varepsilon_F < 0$  one has a sort of  $p$ -doping.

### 3. Hydrodynamical models: general considerations

The macroscopic quantities represent average values of some functions of the wave vector  $\mathbf{k}$  with respect to the distribution function  $f(\mathbf{r}, \mathbf{k}, t)$ . For example, the density  $\rho(\mathbf{r}, t)$  is given by

$$\rho(\mathbf{r}, t) = \frac{2}{(2\pi)^2} \int_{\mathbb{R}^2} f(\mathbf{r}, \mathbf{k}, t) d^2\mathbf{k}.$$

Similarly the average energy  $W(\mathbf{r}, t)$  is given by the relation

$$\rho(\mathbf{r}, t)W(\mathbf{r}, t) = \frac{2}{(2\pi)^2} \int_{\mathbb{R}^2} f(\mathbf{r}, \mathbf{k}, t) \mathcal{E}(\mathbf{k}) d^2\mathbf{k}.$$

Generally speaking, given a weight function  $\psi(\mathbf{k})$ , the corresponding macroscopic quantity is the expectation value

$$M(\mathbf{r}, t) = \frac{2}{(2\pi)^2} \int_{\mathbb{R}^2} \psi(\mathbf{k}) f(\mathbf{r}, \mathbf{k}, t) d^2\mathbf{k}.$$

The evolution equation for  $M(\mathbf{r}, t)$  is deduced by multiplying Eq. (2) for  $\psi(\mathbf{k})$  and by integrating with respect to  $\mathbf{k}$

$$\frac{\partial M}{\partial t} + \nabla_{\mathbf{r}} \cdot \int_{\mathbb{R}^2} f \frac{2\psi(\mathbf{k})}{(2\pi)^2} \mathbf{v}(\mathbf{k}) d^2\mathbf{k} - \frac{q}{\hbar} \mathbf{E} \cdot \int_{\mathbb{R}^2} f \nabla_{\mathbf{k}} \frac{2\psi(\mathbf{k})}{(2\pi)^2} d^2\mathbf{k} = \int_{\mathbb{R}^2} \frac{2\psi(\mathbf{k})}{(2\pi)^2} C[f] d^2\mathbf{k}. \quad (8)$$

Note that the moment equations only depend from the independent variables  $\mathbf{r}, t$ . This reduces noticeably the numerical complexity.

The macroscopic models differs for the different expressions of  $\psi(\mathbf{k})$  employed in the moment equations, e.g. the drift-diffusion models only use the balance equation for the density while the energy-transport models utilize, in addition, the balance equation for energy. In analogy with fluid-dynamics, we talk about hydrodynamical models if at least the balance equations for density, velocity and energy are included.

The main issue related to any model based on balance equations deduced as moment equations of the type (8) is the fact that more unknowns than the introduced moments are present in the evolution equations, and the so-called *closure problem* arises. The latter amounts in expressing the additional unknowns, that are the extra fluxes and the production terms

$$\int_{\mathbb{R}^2} f \frac{2\psi(\mathbf{k})}{(2\pi)^2} \mathbf{v}(\mathbf{k}) d^2\mathbf{k}, \quad \int_{\mathbb{R}^2} f \nabla_{\mathbf{k}} \frac{2\psi(\mathbf{k})}{(2\pi)^2} d^2\mathbf{k}, \quad \int_{\mathbb{R}^2} \frac{2\psi(\mathbf{k})}{(2\pi)^2} C[f] d^2\mathbf{k},$$

as functions of the basic moments.

A systematic way to get the needed closure relations is by employing the Maximum Entropy Principle (MEP). It is based on the information theory of Shannon and was devised for application in statistical physics by Jaynes (1957) (for a general review of the application of MEP to semiconductors the interested reader can refer to Mascali and Romano (2017b)). The distribution obtained with MEP is the least biased estimator under the knowledge of a finite number of expectation values.

Let us suppose that a certain number of moments  $M_A(\mathbf{r}, t)$ ,  $A = 1, 2, \dots, N$ , relative to the weight functions  $\psi_A(\mathbf{k})$ , are known. According to MEP the electron distribution

function is estimated with the distribution  $f_{MEP}$  obtained solving the following constrained optimization problem: for fixed  $\mathbf{r}$  and  $t$ ,

$$\begin{aligned} \max_{f \in \mathcal{F}} S[f] \quad & \text{under the constraints} \\ 0 < f < 1, \end{aligned} \quad (9)$$

$$M_A = \frac{2}{(2\pi)^2} \int_{\mathbb{R}^2} \psi_A(\mathbf{k}) f(\mathbf{r}, \mathbf{k}, t) d^2 \mathbf{k}, \quad A = 1, 2, \dots, N, \quad (10)$$

where  $S[f]$  is the entropy of the system, which reads

$$S[f] = -2 \frac{2k_B}{(2\pi)^2} \int_{\mathbb{R}^2} [f \ln f + (1-f) \ln(1-f)] d^2 \mathbf{k}.$$

The factor 2 takes into account the degeneracy of the valleys. We recall that  $\mathcal{F}$  is the space of the function  $g(\mathbf{k})$  such that  $\psi_A(\mathbf{k})g(\mathbf{k}) \in L^1(\mathbb{R}^2)$  for  $A = 1, 2, \dots, N$ .

Here with  $L^1(\mathbb{R}^2)$  we have denoted the usual Banach space of the summable functions defined over  $\mathbb{R}^2$ .

In order to take into account the bilateral constraints let us introduce the Lagrange multipliers  $\lambda_A$ ,  $A = 1, 2, \dots, N$ , and the Legendre transform of  $S$

$$S' = S + \sum_A \lambda_A \left( M_A - \frac{2}{(2\pi)^2} \int_{\mathbb{R}^2} f \psi_A(\mathbf{k}) d^2 \mathbf{k} \right).$$

The optimality condition  $\delta S' = 0$  gives

$$f_{MEP}(\mathbf{r}, \mathbf{k}, t) = \frac{1}{1 + \exp[\sum_A \psi_A(\mathbf{k}) \lambda_A(\mathbf{r}, t)]},$$

which also fulfils the unilateral constraints (9).

The multiplicative constant  $1/(2k_B)$  has been included into the multipliers for the sake of simplicity the notation.

To complete the optimization procedure it is necessary to invert the relations (10) and express the Lagrangian multipliers as functions of the basic variables. In general this can be achieved only numerically or under some approximation, e.g. expanding around the equilibrium state.

Once the above mentioned problem of the inversion is solved in some way and  $f_{MEP}$  is gotten, the needed closure relations are obtained evaluating the extra fluxes and production terms with  $f_{MEP}$  instead of  $f$ .

The goodness of the models obtained with different choices of the basic moments can be assessed *a posteriori* by a comparison with the results obtained through a direct integration of the transport equation (2).

#### 4. An 8-moment model with the flux of the square power of energy

Camiola and Romano (2014) formulated a 6-moment model by taking as fundamental variables the electron density, linear momentum, energy and energy flux, similarly to what done by Romano (2007), Romano and Zwierz (2010), Camiola *et al.* (2011), Mascali and Romano (2011), Ali *et al.* (2012), Camiola *et al.* (2013), Muscato and Stefano (2013), Mascali (2015, 2016), and Mascali and Romano (2017a) for silicon and gallium arsenide. In this paper we investigate an 8-moment model by including additional moments which are

averages involving higher powers of energy. Explicitly, we consider the following weight functions  $\{1, \mathcal{E}(\mathbf{k}), v, \mathcal{E}(\mathbf{k})v(\mathbf{k}), \mathcal{E}^2(\mathbf{k})v(\mathbf{k})\}$  to which the following moments

$$\rho = \frac{2}{(2\pi)^2} \int_{\mathbb{R}^2} f(\mathbf{r}, \mathbf{k}, t) d^2\mathbf{k}, \quad (11)$$

$$\rho W = 1 \frac{2}{(2\pi)^2} \int_{\mathbb{R}^2} f(\mathbf{r}, \mathbf{k}, t) \mathcal{E}(\mathbf{k}) d^2\mathbf{k}, \quad (12)$$

$$\rho \mathbf{V} = \frac{2}{(2\pi)^2} \int_{\mathbb{R}^2} f(\mathbf{r}, \mathbf{k}, t) \mathbf{v}(\mathbf{k}) d^2\mathbf{k}, \quad (13)$$

$$\rho \mathbf{S} = \frac{2}{(2\pi)^2} \int_{\mathbb{R}^2} f(\mathbf{r}, \mathbf{k}, t) \mathcal{E}(\mathbf{k}) \mathbf{v}(\mathbf{k}) d^2\mathbf{k}, \quad (14)$$

$$\rho \mathbf{S}^{(2)} = \frac{2}{(2\pi)^2} \int_{\mathbb{R}^2} f(\mathbf{r}, \mathbf{k}, t) \mathcal{E}^2(\mathbf{k}) \mathbf{v}(\mathbf{k}) d^2\mathbf{k} \quad (15)$$

correspond. Their evolution equations are obtained by taking the moments of the Boltzmann equation with respect to the same set of weight functions and read

$$\frac{\partial}{\partial t} \rho + \nabla_{\mathbf{r}} \cdot (\rho \mathbf{V}) = \rho C_{\rho}, \quad (16)$$

$$\frac{\partial}{\partial t} (\rho W) + \nabla_{\mathbf{r}} \cdot (\rho \mathbf{S}) + q\rho \mathbf{E} \cdot \mathbf{V} = \rho C_W, \quad (17)$$

$$\frac{\partial}{\partial t} (\rho \mathbf{V}) + \nabla_{\mathbf{r}} \cdot (\rho \mathbf{F}^{(0)}) + q\rho \mathbf{G}^{(0)} : \mathbf{E} = \rho C_{\mathbf{V}}, \quad (18)$$

$$\frac{\partial}{\partial t} (\rho \mathbf{S}) + \nabla_{\mathbf{r}} \cdot (\rho \mathbf{F}^{(1)}) + q\rho \mathbf{G}^{(1)} : \mathbf{E} = \rho C_{\mathbf{S}}, \quad (19)$$

$$\frac{\partial}{\partial t} (\rho \mathbf{S}^{(2)}) + \nabla_{\mathbf{r}} \cdot (\rho \mathbf{F}^{(2)}) + q\rho \mathbf{G}^{(2)} : \mathbf{E} = \rho C_{\mathbf{S}^{(2)}}. \quad (20)$$

The additional quantities, appearing in the previous balance equations and must be expressed in terms of  $\rho, W, \mathbf{V}, \mathbf{S}, \mathbf{S}^{(2)}$ , are the production terms

$$\rho C_{\rho} = \frac{2}{(2\pi)^2} \int_{\mathbb{R}^2} C(\mathbf{k}) d^2\mathbf{k}, \quad (21)$$

$$\rho C_W = \frac{2}{(2\pi)^2} \int_{\mathbb{R}^2} \mathcal{E}(\mathbf{k}) C(\mathbf{k}) d^2\mathbf{k}, \quad (22)$$

$$\rho C_{\mathbf{V}} = \frac{2}{(2\pi)^2} \int_{\mathbb{R}^2} \mathbf{v}(\mathbf{k}) C(\mathbf{k}) d^2\mathbf{k}, \quad (23)$$

$$\rho C_{\mathbf{S}} = \frac{2}{(2\pi)^2} \int_{\mathbb{R}^2} \mathcal{E}(\mathbf{k}) \mathbf{v}(\mathbf{k}) C(\mathbf{k}) d^2\mathbf{k}, \quad (24)$$

$$\rho C_{\mathbf{S}^{(2)}} = \frac{2}{(2\pi)^2} \int_{\mathbb{R}^2} \mathcal{E}^2(\mathbf{k}) \mathbf{v}(\mathbf{k}) C(\mathbf{k}) d^2\mathbf{k}, \quad (25)$$

and the fluxes<sup>1</sup>

$$\rho \mathbf{G}^{(0)} = \frac{2}{\hbar (2\pi)^2} \int_{\mathbb{R}^2} f(\mathbf{r}, \mathbf{k}, t) \nabla_{\mathbf{k}} \mathbf{v}(\mathbf{k}) d^2\mathbf{k}, \quad (26)$$

<sup>1</sup>The symbol  $\otimes$  denotes the tensor product of vectors

$$\rho \mathbf{G}^{(1)} = \frac{2}{\hbar (2\pi)^2} \int_{\mathbb{R}^2} f(\mathbf{r}, \mathbf{k}, t) \nabla_{\mathbf{k}}(\mathcal{E}(\mathbf{k}) \mathbf{v}(\mathbf{k})) d^2 \mathbf{k}, \quad (27)$$

$$\rho \mathbf{G}^{(2)} = \frac{2}{\hbar (2\pi)^2} \int_{\mathbb{R}^2} f(\mathbf{r}, \mathbf{k}, t) \nabla_{\mathbf{k}}(\mathcal{E}^2(\mathbf{k}) \mathbf{v}(\mathbf{k})) d^2 \mathbf{k}, \quad (28)$$

$$\rho \mathbf{F}^{(0)} = \frac{2}{(2\pi)^2} \int_{\mathbb{R}^2} \mathbf{v}(\mathbf{k}) \otimes \mathbf{v}(\mathbf{k}) f(\mathbf{r}, \mathbf{k}, t) d^2 \mathbf{k}, \quad (29)$$

$$\rho \mathbf{F}^{(1)} = \frac{2}{(2\pi)^2} \int_{\mathbb{R}^2} \mathcal{E}(\mathbf{k}) \mathbf{v}(\mathbf{k}) \otimes \mathbf{v}(\mathbf{k}) f(\mathbf{r}, \mathbf{k}, t) d^2 \mathbf{k}, \quad (30)$$

$$\rho \mathbf{F}^{(2)} = \frac{2}{(2\pi)^2} \int_{\mathbb{R}^2} \mathcal{E}^2(\mathbf{k}) \mathbf{v}(\mathbf{k}) \otimes \mathbf{v}(\mathbf{k}) f(\mathbf{r}, \mathbf{k}, t) d^2 \mathbf{k}. \quad (31)$$

Regarding the production terms, they are given by the sum of contributions arising from the different types of phonon scattering

$$\rho C_M = \rho C_M^{(ac)} + \sum_{s=LO,TO,K} \rho C_M^{(s)}$$

with  $M = \rho, W, \mathbf{V}, \mathbf{S}, \mathbf{S}^{(2)}$ .

**4.1. Closure relations.** By exploiting MEP, the following estimator of the distribution function is obtained

$$f_{MEP}(\mathbf{r}, \mathbf{k}, t) = \frac{1}{1 + \exp\left(\lambda(\mathbf{r}, t) + \lambda_w(\mathbf{r}, t) \mathcal{E}(\mathbf{k}) + (\lambda_{\mathbf{V}}(\mathbf{r}, t) + \mathcal{E}(\mathbf{k}) \lambda_{\mathbf{S}}(\mathbf{r}, t) + \mathcal{E}^2(\mathbf{k}) \lambda_{\mathbf{S}^{(2)}}(\mathbf{r}, t)) \cdot \mathbf{v}(\mathbf{k})\right)}, \quad (32)$$

where  $\lambda, \lambda_w, \lambda_{\mathbf{S}}, \lambda_{\mathbf{S}^{(2)}}$  are the set of Lagrange multipliers relative to the basic fields.

If one linearizes by considering the vectorial quantities as first order terms because they vanish at equilibrium, the MEP estimator can be written as <sup>2</sup>

$$f_{MEP}(\mathbf{r}, \mathbf{k}, t) \approx \frac{1}{1 + e^{\lambda + \lambda_w \mathcal{E}}} - \frac{e^{\lambda + \lambda_w \mathcal{E}}}{(1 + e^{\lambda + \lambda_w \mathcal{E}})^2} (\lambda_{\mathbf{V}} + \mathcal{E} \lambda_{\mathbf{S}} + \mathcal{E}^2 \lambda_{\mathbf{S}^{(2)}}) \cdot \mathbf{v}. \quad (33)$$

This is the expression we will use in the following.

We choose a reference frame  $(\mathbf{e}_1, \mathbf{e}_2)$  so that  $\lambda_{\mathbf{V}} = \lambda_{\mathbf{V}} \mathbf{e}_1$ ,  $\lambda_{\mathbf{S}} = \lambda_{\mathbf{S}} \mathbf{e}_1$ ,  $\lambda_{\mathbf{S}^{(2)}} = \lambda_{\mathbf{S}^{(2)}} \mathbf{e}_1$ ,  $\mathbf{E} = E \mathbf{e}_1$ ,  $\mathbf{v} = v_F \cos \phi \mathbf{e}_1 + v_F \sin \phi \mathbf{e}_2$ .

The relations between fields and Lagrange multipliers are given by

$$\rho = \frac{1}{\pi \hbar^2 v_F^2} \int_0^{+\infty} \frac{\mathcal{E}}{1 + e^{\lambda + \lambda_w \mathcal{E}}} d\mathcal{E}, \quad (34)$$

$$\rho W = \frac{1}{\pi \hbar^2 v_F^2} \int_0^{+\infty} \frac{\mathcal{E}^2}{1 + e^{\lambda + \lambda_w \mathcal{E}}} d\mathcal{E}, \quad (35)$$

$$\begin{aligned} \rho \mathbf{V} &= -\frac{1}{2\pi \hbar^2} \int_0^{+\infty} \frac{\mathcal{E} e^{\lambda + \lambda_w \mathcal{E}}}{(1 + e^{\lambda + \lambda_w \mathcal{E}})^2} (\lambda_{\mathbf{V}} + \mathcal{E} \lambda_{\mathbf{S}} + \mathcal{E}^2 \lambda_{\mathbf{S}^{(2)}}) d\mathcal{E} = \\ &= -\frac{1}{2\pi \hbar^2} \left\{ \int_0^{+\infty} \frac{\mathcal{E} e^{\lambda + \lambda_w \mathcal{E}}}{(1 + e^{\lambda + \lambda_w \mathcal{E}})^2} d\mathcal{E} \lambda_{\mathbf{V}} + \int_0^{+\infty} \frac{\mathcal{E}^2 e^{\lambda + \lambda_w \mathcal{E}}}{(1 + e^{\lambda + \lambda_w \mathcal{E}})^2} d\mathcal{E} \lambda_{\mathbf{S}} \right. \end{aligned}$$

<sup>2</sup>The explicit dependence on  $\mathbf{r}, \mathbf{k}, t$  is omitted for the sake of simplifying the notation.

$$+ \int_0^{+\infty} \frac{\mathcal{E}^3 e^{\lambda+\lambda_w \mathcal{E}}}{(1+e^{\lambda+\lambda_w \mathcal{E}})^2} d\mathcal{E} \lambda_{\mathbf{S}}^{(2)} \Big\} \tag{36}$$

$$\begin{aligned} \rho_{\mathbf{S}} = & -\frac{1}{2\pi\hbar^2} \int_0^{+\infty} \frac{\mathcal{E}^2 e^{\lambda+\lambda_w \mathcal{E}}}{(1+e^{\lambda+\lambda_w \mathcal{E}})^2} (\lambda_{\mathbf{V}} + \mathcal{E} \lambda_{\mathbf{S}} + \mathcal{E}^2 \lambda_{\mathbf{S}}^{(2)}) d\mathcal{E} = \\ & -\frac{1}{2\pi\hbar^2} \left\{ \int_0^{+\infty} \frac{\mathcal{E}^2 e^{\lambda+\lambda_w \mathcal{E}}}{(1+e^{\lambda+\lambda_w \mathcal{E}})^2} d\mathcal{E} \lambda_{\mathbf{V}} + \int_0^{+\infty} \frac{\mathcal{E}^3 e^{\lambda+\lambda_w \mathcal{E}}}{(1+e^{\lambda+\lambda_w \mathcal{E}})^2} d\mathcal{E} \lambda_{\mathbf{S}} \right. \\ & \left. + \int_0^{+\infty} \frac{\mathcal{E}^4 e^{\lambda+\lambda_w \mathcal{E}}}{(1+e^{\lambda+\lambda_w \mathcal{E}})^2} d\mathcal{E} \lambda_{\mathbf{S}}^{(2)} \right\}, \end{aligned} \tag{37}$$

$$\begin{aligned} \rho_{\mathbf{S}}^{(2)} = & -\frac{1}{2\pi\hbar^2} \int_0^{+\infty} \frac{\mathcal{E}^3 e^{\lambda+\lambda_w \mathcal{E}}}{(1+e^{\lambda+\lambda_w \mathcal{E}})^2} (\lambda_{\mathbf{V}} + \mathcal{E} \lambda_{\mathbf{S}} + \mathcal{E}^2 \lambda_{\mathbf{S}}^{(2)}) d\mathcal{E} = \\ & -\frac{1}{2\pi\hbar^2} \left\{ \int_0^{+\infty} \frac{\mathcal{E}^3 e^{\lambda+\lambda_w \mathcal{E}}}{(1+e^{\lambda+\lambda_w \mathcal{E}})^2} d\mathcal{E} \lambda_{\mathbf{V}} + \int_0^{+\infty} \frac{\mathcal{E}^4 e^{\lambda+\lambda_w \mathcal{E}}}{(1+e^{\lambda+\lambda_w \mathcal{E}})^2} d\mathcal{E} \lambda_{\mathbf{S}} \right. \\ & \left. + \int_0^{+\infty} \frac{\mathcal{E}^5 e^{\lambda+\lambda_w \mathcal{E}}}{(1+e^{\lambda+\lambda_w \mathcal{E}})^2} d\mathcal{E} \lambda_{\mathbf{S}}^{(2)} \right\}. \end{aligned} \tag{38}$$

These relations have been obtained by writing the wave vector  $\mathbf{k}$  in terms of energy  $\mathcal{E}$  and the angle  $\phi$ .

Regarding the relevant components of fluxes we have

$$\begin{aligned} \rho_{F_{11}}^{(0)} &= \frac{2}{(2\pi)^2} \int_{\mathbb{R}^2} v_1 v_1 f_{MEP}(\mathbf{r}, \mathbf{k}, t) d^2 \mathbf{k} \\ &= \frac{2v_F^2}{(2\pi\hbar v_F)^2} \int_0^{2\pi} d\phi \int_0^{+\infty} \mathcal{E} d\mathcal{E} \cos^2 \phi f_{MEP}(\mathbf{r}, \mathbf{k}, t) \\ &\approx \frac{2\pi v_F^2}{(2\pi\hbar v_F)^2} \left\{ \int_0^{+\infty} \frac{\mathcal{E}}{1+e^{\lambda+\lambda_w \mathcal{E}}} d\mathcal{E} \right\}, \end{aligned} \tag{39}$$

$$\begin{aligned} \rho_{F_{11}}^{(1)} &= \frac{2}{(2\pi)^2} \int_{\mathbb{R}^2} \mathcal{E} v_1 v_1 f_{MEP}(\mathbf{r}, \mathbf{k}, t) d^2 \mathbf{k} \\ &= \frac{2v_F^2}{(2\pi\hbar v_F)^2} \int_0^{2\pi} d\phi \int_0^{+\infty} \mathcal{E}^2 d\mathcal{E} \cos^2 \phi f_{MEP}(\mathbf{r}, \mathbf{k}, t) \\ &\approx \frac{2\pi v_F^2}{(2\pi\hbar v_F)^2} \left\{ \int_0^{+\infty} \frac{\mathcal{E}^2}{1+e^{\lambda+\lambda_w \mathcal{E}}} d\mathcal{E} \right\}, \end{aligned} \tag{40}$$

$$\begin{aligned} \rho_{F_{11}}^{(2)} &= \frac{2}{(2\pi)^2} \int_{\mathbb{R}^2} \mathcal{E}^2 v_1 v_1 f_{MEP}(\mathbf{r}, \mathbf{k}, t) d^2 \mathbf{k} \\ &= \frac{2v_F^2}{(2\pi\hbar v_F)^2} \int_0^{2\pi} d\phi \int_0^{+\infty} \mathcal{E}^3 d\mathcal{E} \cos^2 \phi f_{MEP}(\mathbf{r}, \mathbf{k}, t) \\ &\approx \frac{2\pi v_F^2}{(2\pi\hbar v_F)^2} \left\{ \int_0^{+\infty} \frac{\mathcal{E}^3}{1+e^{\lambda+\lambda_w \mathcal{E}}} d\mathcal{E} \right\}, \end{aligned} \tag{41}$$

$$\rho F_{12}^{(0)} = \frac{2}{(2\pi)^2} \int_{\mathbb{R}^2} v_1 v_2 f_{MEP}(\mathbf{r}, \mathbf{k}, t) d^2 \mathbf{k} \approx 0, \quad (42)$$

$$\rho F_{12}^{(1)} = \frac{2}{(2\pi)^2} \int_{\mathbb{R}^2} \mathcal{E} v_1 v_2 f_{MEP}(\mathbf{r}, \mathbf{k}, t) d^2 \mathbf{k} \approx 0, \quad (43)$$

$$\rho F_{12}^{(2)} = \frac{2}{(2\pi)^2} \int_{\mathbb{R}^2} \mathcal{E}^2 v_1 v_2 f_{MEP}(\mathbf{r}, \mathbf{k}, t) d^2 \mathbf{k} \approx 0, \quad (44)$$

$$\begin{aligned} \rho F_{22}^{(0)} &= \frac{2}{(2\pi)^2} \int_{\mathbb{R}^2} v_2 v_2 f_{MEP}(\mathbf{r}, \mathbf{k}, t) d^2 \mathbf{k} \\ &= \frac{2v_F^2}{(2\pi\hbar v_F)^2} \int_0^{2\pi} d\phi \int_0^{+\infty} \mathcal{E} d\mathcal{E} \sin^2 \phi f_{MEP}(\mathbf{r}, \mathbf{k}, t) \\ &\approx \frac{2\pi v_F^2}{(2\pi\hbar v_F)^2} \left\{ \int_0^{+\infty} \frac{\mathcal{E}}{1 + e^{\lambda + \lambda_w \mathcal{E}}} d\mathcal{E} \right\}, \end{aligned} \quad (45)$$

$$\begin{aligned} \rho F_{22}^{(1)} &= \frac{2}{(2\pi)^2} \int_{\mathbb{R}^2} \mathcal{E} v_2 v_2 f_{MEP}(\mathbf{r}, \mathbf{k}, t) d^2 \mathbf{k} \\ &= \frac{2v_F^2}{(2\pi\hbar v_F)^2} \int_0^{2\pi} d\phi \int_0^{+\infty} \mathcal{E}^2 d\mathcal{E} \sin^2 \phi f_{MEP}(\mathbf{r}, \mathbf{k}, t) \\ &\approx \frac{2\pi v_F^2}{(2\pi\hbar v_F)^2} \left\{ \int_0^{+\infty} \frac{\mathcal{E}^2}{1 + e^{\lambda + \lambda_w \mathcal{E}}} d\mathcal{E} \right\}, \end{aligned} \quad (46)$$

$$\begin{aligned} \rho F_{22}^{(2)} &= \frac{2}{(2\pi)^2} \int_{\mathbb{R}^2} \mathcal{E}^2 v_2 v_2 f_{MEP}(\mathbf{r}, \mathbf{k}, t) d^2 \mathbf{k} \\ &= \frac{2v_F^2}{(2\pi\hbar v_F)^2} \int_0^{2\pi} d\phi \int_0^{+\infty} \mathcal{E}^3 d\mathcal{E} \sin^2 \phi f_{MEP}(\mathbf{r}, \mathbf{k}, t) \\ &\approx \frac{2\pi v_F^2}{(2\pi\hbar v_F)^2} \left\{ \int_0^{+\infty} \frac{\mathcal{E}^3}{1 + e^{\lambda + \lambda_w \mathcal{E}}} d\mathcal{E} \right\}, \end{aligned} \quad (47)$$

where  $v_i$  are the components of  $\mathbf{v}$ .

The drift terms are estimated as follows

$$\rho \mathbf{G}^{(0)} : E \mathbf{e}_1 = \rho G_{11}^{(0)} E = \frac{E}{2\hbar^2 \pi} \left\{ \int_0^{+\infty} \frac{1}{1 + e^{\lambda + \lambda_w \mathcal{E}}} d\mathcal{E} \right\}, \quad (48)$$

$$\rho \mathbf{G}^{(1)} : E \mathbf{e}_1 = \rho G_{11}^{(1)} E = \frac{E}{\hbar^2 \pi} \left\{ \int_0^{+\infty} \frac{\mathcal{E}}{1 + e^{\lambda + \lambda_w \mathcal{E}}} d\mathcal{E} \right\}, \quad (49)$$

$$\rho \mathbf{G}^{(2)} : E \mathbf{e}_1 = \rho G_{11}^{(2)} E = \frac{3E}{2\hbar^2 \pi} \left\{ \int_0^{+\infty} \frac{\mathcal{E}^2}{1 + e^{\lambda + \lambda_w \mathcal{E}}} d\mathcal{E} \right\}. \quad (50)$$

**4.2. Production terms.** Regarding the production terms, the estimators listed below are obtained.

The productions arising from the scattering with acoustic phonons are given by

$$\rho C_p^{(ac)} = 0, \quad (51)$$

$$\rho C_W^{(ac)} = 0, \quad (52)$$

$$\rho C_V^{(ac)} = \frac{1}{8\pi^2 \hbar^4 v_F^2} A^{(ac)} \left\{ \int_0^{+\infty} \frac{\mathcal{E}^2 e^{\lambda + \lambda_w \mathcal{E}}}{(1 + e^{\lambda + \lambda_w \mathcal{E}})^2} (\lambda_V + \mathcal{E} \lambda_S + \mathcal{E}^2 \lambda_S^{(2)}) d\mathcal{E} \right\}, \quad (53)$$

$$\rho C_S^{(ac)} = \frac{1}{8\pi^2 \hbar^4 v_F^2} A^{(ac)} \left\{ \int_0^{+\infty} \frac{\mathcal{E}^3 e^{\lambda + \lambda_w \mathcal{E}}}{(1 + e^{\lambda + \lambda_w \mathcal{E}})^2} (\lambda_V + \mathcal{E} \lambda_S + \mathcal{E}^2 \lambda_S^{(2)}) d\mathcal{E} \right\}, \quad (54)$$

$$\rho C_{S^{(2)}}^{(ac)} = \frac{1}{8\pi^2 \hbar^4 v_F^2} A^{(ac)} \left\{ \int_0^{+\infty} \frac{\mathcal{E}^4 e^{\lambda + \lambda_w \mathcal{E}}}{(1 + e^{\lambda + \lambda_w \mathcal{E}})^2} (\lambda_V + \mathcal{E} \lambda_S + \mathcal{E}^2 \lambda_S^{(2)}) d\mathcal{E} \right\}. \quad (55)$$

If we set  $\beta = \frac{1}{k_B T_L}$ , the productions arising from the scattering with optical phonons read

$$\rho C_\rho^{(OP)} = 0, \quad (56)$$

$$\rho C_W^{(OP)} = \frac{A^{OP} D_K^2 N_B^{OP}}{\hbar^4 v_F^4 \pi^2} \hbar \omega (e^{\lambda_w \hbar \omega} - e^{\beta \hbar \omega}) \int_0^{+\infty} f^{(i)}(\mathcal{E} + \hbar \omega) \left( \frac{e^{\lambda + \lambda_w \mathcal{E}}}{1 + e^{\lambda + \lambda_w \mathcal{E}}} \right) \mathcal{E} (\mathcal{E} + \hbar \omega) d\mathcal{E}, \quad (57)$$

$$\begin{aligned} \rho C_V^{(OP)} &= \frac{A^{OP} D_K^2 N_B^{OP}}{2\hbar^4 v_F^2 \pi^2} \left\{ \int_0^{+\infty} \left( \frac{e^{\lambda + \lambda_w (\mathcal{E} + \hbar \omega)}}{(1 + e^{\lambda + \lambda_w (\mathcal{E} + \hbar \omega)})^2} (\lambda_V + (\mathcal{E} + \hbar \omega) \lambda_S + (\mathcal{E} + \hbar \omega)^2 \lambda_S^{(2)}) \right) \mathcal{E} (\mathcal{E} + \hbar \omega) \right. \\ &\quad \times \left[ f^{(i)}(\mathcal{E}) + (1 - f^{(i)}(\mathcal{E})) e^{\beta \hbar \omega} \right] d\mathcal{E} + \int_0^{+\infty} \left( \frac{e^{\lambda + \lambda_w \mathcal{E}}}{(1 + e^{\lambda + \lambda_w \mathcal{E}})^2} (\lambda_V + \mathcal{E} \lambda_S + \mathcal{E}^2 \lambda_S^{(2)}) \right) \mathcal{E} (\mathcal{E} + \hbar \omega) \\ &\quad \left. \times \left[ e^{\beta \hbar \omega} f^{(i)}(\mathcal{E} + \hbar \omega) + (1 - f^{(i)}(\mathcal{E} + \hbar \omega)) \right] d\mathcal{E} \right\}, \quad (58) \end{aligned}$$

$$\begin{aligned} \rho C_S^{(OP)} &= \frac{A^{OP} D_K^2 N_B^{OP}}{2\hbar^4 v_F^2 \pi^2} \left\{ \int_0^{+\infty} \left( \frac{e^{\lambda + \lambda_w (\mathcal{E} + \hbar \omega)}}{(1 + e^{\lambda + \lambda_w (\mathcal{E} + \hbar \omega)})^2} (\lambda_V + (\mathcal{E} + \hbar \omega) \lambda_S + (\mathcal{E} + \hbar \omega)^2 \lambda_S^{(2)}) \right) \mathcal{E} (\mathcal{E} + \hbar \omega)^2 \right. \\ &\quad \times \left[ f^{(i)}(\mathcal{E}) + (1 - f^{(i)}(\mathcal{E})) e^{\beta \hbar \omega} \right] d\mathcal{E} + \int_0^{+\infty} \left( \frac{e^{\lambda + \lambda_w \mathcal{E}}}{(1 + e^{\lambda + \lambda_w \mathcal{E}})^2} (\lambda_V + \mathcal{E} \lambda_S + \mathcal{E}^2 \lambda_S^{(2)}) \right) (\mathcal{E} + \hbar \omega) \mathcal{E}^2 \\ &\quad \left. \times \left[ e^{\beta \hbar \omega} f^{(i)}(\mathcal{E} + \hbar \omega) + (1 - f^{(i)}(\mathcal{E} + \hbar \omega)) \right] d\mathcal{E} \right\}, \quad (59) \end{aligned}$$

$$\begin{aligned} \rho C_{S^{(2)}}^{(OP)} &= \frac{A^{OP} D_K^2 N_B^{OP}}{2\hbar^4 v_F^2 \pi^2} \left\{ \int_0^{+\infty} \left( \frac{e^{\lambda + \lambda_w (\mathcal{E} + \hbar \omega)}}{(1 + e^{\lambda + \lambda_w (\mathcal{E} + \hbar \omega)})^2} (\lambda_V + (\mathcal{E} + \hbar \omega) \lambda_S + (\mathcal{E} + \hbar \omega)^2 \lambda_S^{(2)}) \right) \mathcal{E} (\mathcal{E} + \hbar \omega)^3 \right. \\ &\quad \times \left[ f^{(i)}(\mathcal{E}) + (1 - f^{(i)}(\mathcal{E})) e^{\beta \hbar \omega} \right] d\mathcal{E} + \int_0^{+\infty} \left( \frac{e^{\lambda + \lambda_w \mathcal{E}}}{(1 + e^{\lambda + \lambda_w \mathcal{E}})^2} (\lambda_V + \mathcal{E} \lambda_S + \mathcal{E}^2 \lambda_S^{(2)}) \right) (\mathcal{E} + \hbar \omega) \mathcal{E}^3 \\ &\quad \left. \times \left[ e^{\beta \hbar \omega} f^{(i)}(\mathcal{E} + \hbar \omega) + (1 - f^{(i)}(\mathcal{E} + \hbar \omega)) \right] d\mathcal{E} \right\}. \quad (60) \end{aligned}$$

The productions arising from the scattering with K-phonons can be written as

$$\rho C_\rho^{(K)} = 0, \quad (61)$$

$$\rho C_W^{(K)} = \frac{A^K D_K^2 N_B^K}{2\hbar^4 v_F^4 \pi^2} (e^{\lambda_w \hbar \omega} - e^{\beta \hbar \omega}) \hbar \omega \int_0^{+\infty} f^{(i)}(\mathcal{E}) \left( \frac{e^{\lambda + \lambda_w \mathcal{E}}}{1 + e^{\lambda + \lambda_w (\mathcal{E} + \hbar \omega)}} \right) \mathcal{E} (\mathcal{E} + \hbar \omega) d\mathcal{E}, \quad (62)$$

$$\begin{aligned} \rho C_V^{(K)} &= \frac{3A^K D_K^2 N_B^K}{8\pi^2 \hbar^4 v_F^2} \left\{ \int_0^{+\infty} \left( \frac{e^{\lambda + \lambda_w (\mathcal{E} + \hbar \omega)}}{(1 + e^{\lambda + \lambda_w (\mathcal{E} + \hbar \omega)})^2} (\lambda_V + (\mathcal{E} + \hbar \omega) \lambda_S + (\mathcal{E} + \hbar \omega)^2 \lambda_S^{(2)}) \right) \mathcal{E} (\mathcal{E} + \hbar \omega) \right. \\ &\quad \times \left[ f^{(i)}(\mathcal{E}) + (1 - f^{(i)}(\mathcal{E})) e^{\beta \hbar \omega} \right] d\mathcal{E} \\ &\quad + \int_0^{+\infty} \left( \frac{e^{\lambda + \lambda_w \mathcal{E}}}{(1 + e^{\lambda + \lambda_w \mathcal{E}})^2} (\lambda_V + \mathcal{E} \lambda_S + \mathcal{E}^2 \lambda_S^{(2)}) \right) \mathcal{E} (\mathcal{E} + \hbar \omega) \\ &\quad \left. \times \left[ 1 - f^{(i)}(\mathcal{E} + \hbar \omega) + f^{(i)}(\mathcal{E} + \hbar \omega) e^{\beta \hbar \omega} \right] d\mathcal{E} \right\}, \quad (63) \end{aligned}$$

$$\begin{aligned} \rho C_S^{(K)} &= \frac{A^K D_K^2 N_B^K}{8\pi^2 \hbar^4 v_F^2} \left\{ \int_0^{+\infty} (3\mathcal{E} + 2\hbar \omega) \left( \frac{e^{\lambda + \lambda_w (\mathcal{E} + \hbar \omega)}}{(1 + e^{\lambda + \lambda_w (\mathcal{E} + \hbar \omega)})^2} (\lambda_V + (\mathcal{E} + \hbar \omega) \lambda_S + (\mathcal{E} + \hbar \omega)^2 \lambda_S^{(2)}) \right) \mathcal{E} (\mathcal{E} + \hbar \omega) \right. \\ &\quad \left. \times \left[ f^{(i)}(\mathcal{E}) + (1 - f^{(i)}(\mathcal{E})) e^{\beta \hbar \omega} \right] d\mathcal{E} \right\} \end{aligned}$$

$$\begin{aligned}
 & + \int_0^{+\infty} (3\mathcal{E} + \hbar\omega) \left( \frac{e^{\lambda + \lambda_w \mathcal{E}}}{(1 + e^{\lambda + \lambda_w \mathcal{E}})^2} (\lambda_{\mathbf{V}} + \mathcal{E} \lambda_{\mathbf{S}} + \mathcal{E}^2 \lambda_{\mathbf{S}}^{(2)}) \right) \mathcal{E}(\mathcal{E} + \hbar\omega) \\
 & \times \left[ 1 - f^{(i)}(\mathcal{E} + \hbar\omega) + f^{(i)}(\mathcal{E} + \hbar\omega) e^{\beta \hbar \omega} \right] d\mathcal{E} \Big\}, \tag{64}
 \end{aligned}$$

$$\begin{aligned}
 \rho_{\mathbf{S}^{(2)}}^{C(K)} & = \frac{A^K D_K^2 N_B^K}{8\pi^2 \hbar^4 v_F^2} \left\{ \int_0^{+\infty} (2(\mathcal{E} + \hbar\omega)^2 + \mathcal{E}^2) \left( \frac{e^{\lambda + \lambda_w(\mathcal{E} + \hbar\omega)}}{(1 + e^{\lambda + \lambda_w(\mathcal{E} + \hbar\omega)})^2} (\lambda_{\mathbf{V}} + (\mathcal{E} + \hbar\omega) \lambda_{\mathbf{S}} + (\mathcal{E} + \hbar\omega)^2 \lambda_{\mathbf{S}}^{(2)}) \right) \mathcal{E}(\mathcal{E} + \hbar\omega) \right. \\
 & \times \left[ f^{(i)}(\mathcal{E}) + (1 - f^{(i)}(\mathcal{E})) e^{\beta \hbar \omega} \right] d\mathcal{E} \\
 & + \int_0^{+\infty} ((\mathcal{E} + \hbar\omega)^2 + 2\mathcal{E}^2) \left( \frac{e^{\lambda + \lambda_w \mathcal{E}}}{(1 + e^{\lambda + \lambda_w \mathcal{E}})^2} (\lambda_{\mathbf{V}} + \mathcal{E} \lambda_{\mathbf{S}} + \mathcal{E}^2 \lambda_{\mathbf{S}}^{(2)}) \right) \mathcal{E}(\mathcal{E} + \hbar\omega) \\
 & \times \left[ 1 - f^{(i)}(\mathcal{E} + \hbar\omega) + f^{(i)}(\mathcal{E} + \hbar\omega) e^{\beta \hbar \omega} \right] d\mathcal{E} \Big\}. \tag{65}
 \end{aligned}$$

**5. Mathematical properties of the model with 8 moments**

Before investigating the accuracy of the model, we study its main mathematical features. Let us introduce the following quantities

$$J_n(\lambda, \lambda_w) := \int_0^{+\infty} \frac{\mathcal{E}^n e^{\lambda + \lambda_w \mathcal{E}}}{(1 + e^{\lambda + \lambda_w \mathcal{E}})^2} d\mathcal{E}, \quad K_n(\lambda, \lambda_w) := \frac{1}{2\pi \hbar^2 v_F} J_n(\lambda, \lambda_w).$$

**Theorem 5.1.** *There is a local one-to-one correspondence between Lagrange multipliers and field variables.*

*Proof.* Let us introduce the vectors  $\mathbf{U}^{(1)} = (\rho, W)$  and  $\mathbf{U}_l^{(1)} = (\lambda, \lambda_w)$ . The Jacobian matrix is given by

$$B = \frac{\partial(\rho, W)}{\partial(\lambda, \lambda_w)} = -\frac{1}{\pi \hbar^2 v_F^2} \begin{pmatrix} J_1 & J_2 \\ J_2 & J_3 \end{pmatrix}.$$

Let us consider the quadratic form associated to the matrix  $B$

$$g(\xi) = (\xi_1, \xi_2) B (\xi_1, \xi_2)^T \quad \forall \xi = (\xi_1, \xi_2) \in \mathbb{R}^2.$$

One has

$$g(\xi) = -\frac{1}{\pi \hbar^2 v_F^2} \int_0^{+\infty} \frac{\mathcal{E} e^{\lambda + \lambda_w \mathcal{E}}}{(1 + e^{\lambda + \lambda_w \mathcal{E}})^2} (\xi_1 + \mathcal{E} \xi_2)^2 d\mathcal{E}.$$

Since  $\xi_1 + \mathcal{E} \xi_2$  is zero at most in a set of zero measure,  $g$  is negative definite and there is a local one-to-one correspondence between  $\mathbf{U}^{(1)}$  and  $\mathbf{U}_l^{(1)}$ .

Regarding the vectorial fields, one finds

$$\begin{pmatrix} \rho_{\mathbf{V}} \\ \rho_{\mathbf{S}} \\ \rho_{\mathbf{S}^{(2)}} \end{pmatrix} = -\frac{1}{2\pi \hbar^2} \begin{pmatrix} J_1(\lambda, \lambda_w) & J_2(\lambda, \lambda_w) & J_3(\lambda, \lambda_w) \\ J_2(\lambda, \lambda_w) & J_3(\lambda, \lambda_w) & J_4(\lambda, \lambda_w) \\ J_3(\lambda, \lambda_w) & J_4(\lambda, \lambda_w) & J_5(\lambda, \lambda_w) \end{pmatrix} \begin{pmatrix} \lambda_{\mathbf{V}} \\ \lambda_{\mathbf{S}} \\ \lambda_{\mathbf{S}}^{(2)} \end{pmatrix} := C \begin{pmatrix} \lambda_{\mathbf{V}} \\ \lambda_{\mathbf{S}} \\ \lambda_{\mathbf{S}}^{(2)} \end{pmatrix}.$$

Let us consider the quadratic form associated to the matrix  $C$

$$h(\xi) = (\xi_1, \xi_2, \xi_3) C (\xi_1, \xi_2, \xi_3)^T \quad \forall \xi = (\xi_1, \xi_2, \xi_3) \in \mathbb{R}^3.$$

One has

$$h(\xi) = -\frac{1}{2\pi \hbar^2} \int_0^{+\infty} \frac{\mathcal{E} e^{\lambda + \lambda_w \mathcal{E}}}{(1 + e^{\lambda + \lambda_w \mathcal{E}})^2} (\xi_1 + \mathcal{E} \xi_2 + \mathcal{E}^2 \xi_3)^2 d\mathcal{E}.$$

Since  $\xi_1 + \mathcal{E}\xi_2 + \mathcal{E}^2\xi_3$  is zero at most in a set of zero measure,  $h$  is negative definite and there is a local one-to-one correspondence between Lagrange multipliers and field variables.  $\square$

**Theorem 5.2.** *The evolution equations closed with MEP form a hyperbolic system of balance laws in the time direction.*

*Proof.* Thanks to the previous theorem, we can use the Lagrange multipliers as field variables. In term of the Lagrange multipliers the evolution equations become

$$\frac{d}{dt} \begin{pmatrix} \lambda \\ \lambda_w \\ \lambda_V \\ \lambda_S \\ \lambda_S^{(2)} \end{pmatrix} = \begin{pmatrix} B & O_{2 \times 3} \\ O_{3 \times 3} & C \end{pmatrix}^{-1} \mathcal{G}. \tag{66}$$

where

$$\mathcal{G} = \left[ -q\rho \begin{pmatrix} 0 \\ \mathbf{V} \\ \mathbf{G}^{(0)} \\ \mathbf{G}^{(1)} \\ \mathbf{G}^{(2)} \end{pmatrix} \cdot \mathbf{E} + \rho \begin{pmatrix} C_\rho \\ C_W \\ C_V \\ C_S \\ C_S^{(2)} \end{pmatrix} \right]$$

Denoting with  $(x_1, x_2)$  the spatial variables, the evolution equations can be cast in the form

$$\mathcal{A}_0 \frac{\partial \Lambda}{\partial t} + \mathcal{A}_1 \frac{\partial \Lambda}{\partial x_1} + \mathcal{A}_2 \frac{\partial \Lambda}{\partial x_2} = \mathcal{G} \tag{67}$$

where

$$\Lambda = (\lambda, \lambda_w, \lambda_{V_1}, \lambda_{S_1}, \lambda_{S_1^{(2)}}; \lambda_{V_2}, \lambda_{S_2}, \lambda_{S_2^{(2)}})^T,$$

$$\begin{aligned} \mathcal{A}_0 &= \nabla_\Lambda \mathcal{F}_0 \quad \text{with} \quad \mathcal{F}_0 = (\rho, \rho W, \rho V_1, \rho S_1, \rho S_1^{(2)}, \rho V_2, \rho S_2, \rho S_2^{(2)})^T, \\ \mathcal{A}_1 &= \nabla_\Lambda \mathcal{F}_1 \quad \text{with} \quad \mathcal{F}_1 = (\rho V_1, \rho S_1, \rho F_{11}^{(0)}, \rho F_{11}^{(1)}, \rho F_{11}^{(2)}, \rho F_{21}^{(0)}, \rho F_{21}^{(1)}, \rho F_{21}^{(2)})^T, \\ \mathcal{A}_2 &= \nabla_\Lambda \mathcal{F}_2 \quad \text{with} \quad \mathcal{F}_2 = (\rho V_2, \rho S_2, \rho F_{12}^{(0)}, \rho F_{12}^{(1)}, \rho F_{12}^{(2)}, \rho F_{22}^{(0)}, \rho F_{22}^{(1)}, \rho F_{22}^{(2)})^T. \end{aligned}$$

Here  $V_i$  and  $S_i$   $i = 1, 2$  are the components of  $\mathbf{V}$  and  $\mathbf{S}$  and  $F_{ij}^{(0)}, F_{ij}^{(1)}, F_{ij}^{(2)}$   $i, j = 1, 2$  are the components of the tensors  $\mathbf{F}^{(0)}, \mathbf{F}^{(1)}$  and  $\mathbf{F}^{(2)}$  respectively.

We prove that  $\det(\mathcal{A}_0) \neq 0$ . Omitting the dependence on Lagrangian multipliers  $\lambda$  and  $\lambda_w$  for the sake of simplicity, explicitly  $\mathcal{A}_0$  reads

$$\mathcal{A}_0 = \begin{pmatrix} -\frac{2}{v_F} K_1 & -\frac{2}{v_F} K_2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -\frac{2}{v_F} K_2 & -\frac{2}{v_F} K_3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{\partial \rho V_1}{\partial \lambda} & \frac{\partial \rho V_1}{\partial \lambda_w} & -v_F K_1 & -v_F K_2 & -v_F K_3 & 0 & 0 & 0 & 0 \\ \frac{\partial \rho S_1}{\partial \lambda} & \frac{\partial \rho S_1}{\partial \lambda_w} & -v_F K_2 & -v_F K_3 & -v_F K_4 & 0 & 0 & 0 & 0 \\ \frac{\partial \rho S_1^{(2)}}{\partial \lambda} & \frac{\partial \rho S_1^{(2)}}{\partial \lambda_w} & -v_F K_3 & -v_F K_4 & -v_F K_5 & 0 & 0 & 0 & 0 \\ \frac{\partial \rho V_2}{\partial \lambda} & \frac{\partial \rho V_2}{\partial \lambda_w} & 0 & 0 & 0 & -v_F K_1 & -v_F K_2 & -v_F K_3 & 0 \\ \frac{\partial \rho S_2}{\partial \lambda} & \frac{\partial \rho S_2}{\partial \lambda_w} & 0 & 0 & 0 & -v_F K_2 & -v_F K_3 & -v_F K_4 & 0 \\ \frac{\partial \rho S_2^{(2)}}{\partial \lambda} & \frac{\partial \rho S_2^{(2)}}{\partial \lambda_w} & 0 & 0 & 0 & -v_F K_3 & -v_F K_4 & -v_F K_5 & 0 \end{pmatrix}.$$

We can factorize the determinant of  $\mathcal{A}_0$  as

$$\frac{1}{64} \frac{(J_1 J_3 J_5 - J_1 J_4^2 + 2 J_2 J_4 J_3 - J_2^2 J_5 - J_3^3)^2 (J_1 J_3 - J_2^2)}{\pi^8 h^{16} v^4}.$$

Since the two matrix

$$\begin{pmatrix} J_1 & J_2 \\ J_2 & J_3 \end{pmatrix}, \quad \begin{pmatrix} J_1 & J_2 & J_3 \\ J_2 & J_3 & J_4 \\ J_3 & J_4 & J_5 \end{pmatrix}$$

are positive definite, in virtue of theorem 5.1, it follows that  $\det(\mathcal{A}_0) > 0$  for any value of the fields. For arbitrary  $\mathbf{n} = (n_1, n_2)$  belonging to the unit circle of  $\mathbb{R}^2$ , the eigenvalue equation is

$$\det(n_1 \mathcal{A}_1 + n_2 \mathcal{A}_2 - \mu \mathcal{A}_0) = 0$$

which has the following roots:

$$\begin{aligned} \mu_1 &= 0 \quad \text{with multiplicity four,} \\ \mu_{2,3} &= \pm \frac{\sqrt{2}}{2} v_F \quad \text{both with multiplicity two.} \end{aligned}$$

To complete the analysis of the hyperbolicity, we study the rank of the matrix  $M(\mu) = n_1 \mathcal{A}_1 + n_2 \mathcal{A}_2 - \mu \mathcal{A}_0$  which explicitly is given by

$$\begin{pmatrix} \sum_{i=1}^2 n_i \frac{\partial}{\partial \lambda} (\rho V_i) + \frac{2\mu}{v_F} K_1 & \sum_{i=1}^2 n_i \frac{\partial}{\partial \lambda_w} (\rho V_i) + \frac{2\mu}{v_F} K_2 & -n_1 K_1 & -n_1 K_2 & -n_1 K_3 & -n_2 K_1 & -n_2 K_2 & -n_2 K_3 \\ \sum_{i=1}^2 n_i \frac{\partial}{\partial \lambda} (\rho S_i) + \mu \frac{1}{\pi h^2 v_F} J_2 & \sum_{i=1}^2 n_i \frac{\partial}{\partial \lambda_w} (\rho S_i) + \mu \frac{1}{\pi h^2 v_F} J_3 & -n_1 K_2 & -n_1 K_3 & -n_1 K_4 & -n_2 K_2 & -n_2 K_3 & -n_2 K_4 \\ n_1 \frac{\partial}{\partial \lambda} (\rho F_{11}^{(0)}) - \mu \frac{\partial \rho V_1}{\partial \lambda} & n_1 \frac{\partial}{\partial \lambda_w} (\rho F_{11}^{(0)}) - \mu \frac{\partial \rho V_1}{\partial \lambda_w} & \mu K_1 & \mu K_2 & \mu K_3 & 0 & 0 & 0 \\ n_1 \frac{\partial}{\partial \lambda} (\rho F_{11}^{(1)}) - \mu \frac{\partial \rho S_1}{\partial \lambda} & n_1 \frac{\partial}{\partial \lambda_w} (\rho F_{11}^{(1)}) - \mu \frac{\partial \rho S_1}{\partial \lambda_w} & \mu K_2 & \mu K_3 & \mu K_4 & 0 & 0 & 0 \\ n_1 \frac{\partial}{\partial \lambda} (\rho F_{11}^{(2)}) - \mu \frac{\partial \rho S_1^{(2)}}{\partial \lambda} & n_1 \frac{\partial}{\partial \lambda_w} (\rho F_{11}^{(2)}) - \mu \frac{\partial \rho S_1^{(2)}}{\partial \lambda_w} & \mu K_3 & \mu K_4 & \mu K_5 & 0 & 0 & 0 \\ n_2 \frac{\partial}{\partial \lambda} (\rho F_{22}^{(0)}) - \mu \frac{\partial \rho V_2}{\partial \lambda} & n_2 \frac{\partial}{\partial \lambda_w} (\rho F_{22}^{(0)}) - \mu \frac{\partial \rho V_2}{\partial \lambda_w} & 0 & 0 & 0 & \mu K_1 & \mu K_2 & \mu K_3 \\ n_2 \frac{\partial}{\partial \lambda} (\rho F_{22}^{(1)}) - \mu \frac{\partial \rho S_2}{\partial \lambda} & n_2 \frac{\partial}{\partial \lambda_w} (\rho F_{22}^{(1)}) - \mu \frac{\partial \rho S_2}{\partial \lambda_w} & 0 & 0 & 0 & \mu K_2 & \mu K_3 & \mu K_4 \\ n_2 \frac{\partial}{\partial \lambda} (\rho F_{22}^{(2)}) - \mu \frac{\partial \rho S_2^{(2)}}{\partial \lambda} & n_2 \frac{\partial}{\partial \lambda_w} (\rho F_{22}^{(2)}) - \mu \frac{\partial \rho S_2^{(2)}}{\partial \lambda_w} & 0 & 0 & 0 & \mu K_3 & \mu K_4 & \mu K_5 \end{pmatrix}$$

Let us denote by  $m_{ij}$  the generic element of the matrix  $M(\mu)$ .

1. Case  $\mu = 0$ .

By taking into account the fact that  $\rho F_{11}^{(k)} = \rho F_{22}^{(k)}$ ,  $k = 1, 2$ , from the definition of  $J_n$  it follows that the third, fourth and fifth rows of the matrix  $M(0)$  are proportional to the sixth, seventh and eighth rows, respectively. In fact

$$\begin{aligned} n_2(m_{31}, \dots, m_{3j}, \dots, m_{38}) - n_1(m_{61}, \dots, m_{6j}, \dots, m_{68}) &= 0, \\ n_2(m_{41}, \dots, m_{4j}, \dots, m_{48}) - n_1(m_{71}, \dots, m_{7j}, \dots, m_{78}) &= 0, \\ n_2(m_{51}, \dots, m_{5j}, \dots, m_{58}) - n_1(m_{81}, \dots, m_{8j}, \dots, m_{88}) &= 0. \end{aligned}$$

Therefore, the rank is not greater than six. Moreover, the determinant of the minor of order four obtained by eliminating the last four rows and the last four columns is equal to

$$\frac{1}{16} \frac{n_1^4 (J_1 J_3 - J_2^2)^2}{\pi^4 h^8}$$

which is different from zero because we have previously proved that the quantity  $J_1 J_3 - J_2^2$  is positive. Therefore, apart from the case  $\frac{\partial}{\partial \lambda}(\rho F_{11}^{(k)}) = \frac{\partial}{\partial \lambda}(\rho F_{22}^{(k)}) = 0$ ,  $k = 1, 2$ , the rank of  $M(0)$  is four. From a direct verification, the expressions  $\frac{\partial}{\partial \lambda}(\rho F_{11}^{(k)})$  and  $\frac{\partial}{\partial \lambda}(\rho F_{22}^{(k)})$ ,  $k = 1, 2$ , obtained with MEP, are different from zero. Therefore the rank of  $M(0)$  is always four.

2. Case  $\mu = \frac{\sqrt{2}}{2} v_F$ .

By taking into account the fact that  $\rho F_{11}^{(k)} = \rho F_{22}^{(k)}$ ,  $k = 1, 2$ , from the definition of  $J_n$  it follows that the third row of the matrix  $M(\frac{\sqrt{2}}{2} v_F)$  is a linear combination of the first and sixth rows while the fourth is a linear combination of the second and seventh ones. In fact one has

$$\begin{aligned} n_1(m_{31}, \dots, m_{3j}, \dots, m_{38}) + \mu(m_{11}, \dots, m_{1j}, \dots, m_{18}) + n_2(m_{61}, \dots, m_{6j}, \dots, m_{68}) &= 0, \\ n_1(m_{41}, \dots, m_{4j}, \dots, m_{48}) + \mu(m_{21}, \dots, m_{2j}, \dots, m_{28}) + n_2(m_{71}, \dots, m_{7j}, \dots, m_{78}) &= 0. \end{aligned}$$

Moreover, the determinant of the sub-matrix obtained by eliding the first two rows and the first two columns is

$$\frac{1}{512} \frac{v^6 (J_1 J_3 J_5 - J_1 J_4^2 + 2 J_2 J_4 J_3 - J_2^2 J_5 - J_3^3)^2}{\pi^6 h^{12}},$$

which is different from zero because the matrix of  $C$  of theorem 5.1 is positive definite. Therefore the rank of  $M(\frac{\sqrt{2}}{2} v_F)$  is six.

3. Case  $\mu = -\frac{\sqrt{2}}{2} v_F$ . The same considerations of the previous case hold.

□

### 6. Numerical results

In order to assess the validity of the model, we consider the simple case of pristine suspended graphene under a constant electric field  $\mathbf{E}$ . The physical situation we simulate is that of a strip of graphene which is infinitely long in the transversal direction with respect to that of the electric field (see Fig. 1). This allows to look for solutions which are not depending on space and to avoid any effect related to the boundary conditions.

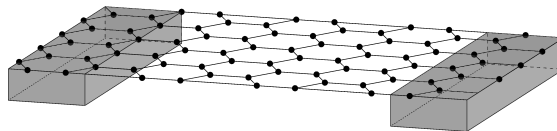


FIGURE 1. Schematic representation of a suspended monolayer graphene. In the direction orthogonal to the contacts the material is infinitely long. In each contact there is a constant electrostatic potential.

The evolution equations are reduced to a system of Ordinary Differential Equations (ODE's). The only significant component of each equation is that along the direction of  $\mathbf{E}$ .

Therefore, the evolution equations read

$$\frac{d}{dt}\rho = 0, \quad (68)$$

$$\frac{d}{dt}(\rho \mathbf{V}) = -q\rho \mathbf{G}^{(0)} : \mathbf{E} + \rho C_V, \quad (69)$$

$$\frac{d}{dt}(\rho W) = -q\rho \mathbf{E} \cdot \mathbf{V} + \rho C_W, \quad (70)$$

$$\frac{d}{dt}(\rho \mathbf{S}) = -q\rho \mathbf{G}^{(1)} : \mathbf{E} + \rho C_S, \quad (71)$$

$$\frac{d}{dt}(\rho \mathbf{S}^{(2)}) = -q\rho \mathbf{G}^{(2)} : \mathbf{E} + \rho C_S^{(2)}. \quad (72)$$

We assume initially thermodynamical equilibrium. As a consequence, the initial conditions for the the macroscopic variables are

$$\rho(0) = \frac{2}{(2\pi)^2} \int_{\mathbb{R}^2} f_{FD}(\mathbf{k}) d^2\mathbf{k}, \quad (73)$$

$$\rho(0)W(0) = \frac{2}{(2\pi)^2} \int_{\mathbb{R}^2} f_{FD}(\mathbf{k}) \mathcal{E} d^2\mathbf{k}, \quad (74)$$

$$\rho(0)\mathbf{V}(0) = \mathbf{0}, \quad (75)$$

$$\rho(0)\mathbf{S}(0) = \mathbf{0}, \quad (76)$$

$$\rho(0)\mathbf{S}^{(2)}(0) = \mathbf{0}. \quad (77)$$

where  $f_{FD}(\mathbf{k})$  is the Fermi-Dirac distribution (7).

The results are plotted in Fig.s 2, 3 for Fermi energy 0.4 eV and in Fig.s 4, 5 for Fermi energy 0.6 eV. We have compared the results obtained with the 8-moment model (8MM) presented in this paper with those obtained with the 6-moment model (6MM) by Camiola and Romano (2014). As reference solutions we have taken those given by a direct numerical integration of the Boltzmann equation with the Discontinuous Galerkin approach proposed by Romano *et al.* (2015) and Coco *et al.* (2016b).

For low electric fields the velocity predicted by 6MM is more accurate than that obtained with 8MM. In the presence of higher electric fields, the difference between 6MM and 8MM is smaller but in any case 6MM performs better or no worse than 8MM. Differences are smaller in energy but again 6MM reveals no worse than 8MM. These considerations do not depend on the Fermi energy. Moreover, the hydrodynamical results systematically overestimate those obtained by the direct solution of the Boltzmann equation. It is likely that this effect is due to an underestimation of the dissipative character of the collision terms.

It is clear that the inclusion of the variable  $\mathbf{S}^{(2)}$  does not improve the model. We have tried to get better results by adding further moments like  $\mathbf{S}^{(3)}$  and  $\mathbf{S}^{(4)}$  (the details are omitted for the sake of conciseness) but from a qualitative point of view no real improvements are obtained. There is a strong numerical evidence that increasing the hierarchy of the field variables with additional terms of the type

$$\rho \mathbf{S}^{(n)} = \frac{2}{(2\pi)^2} \int_{\mathbb{R}^2} f(\mathbf{r}, \mathbf{k}, t) \mathcal{E}^n \mathbf{v} d^2\mathbf{k},$$

with  $n$  a positive integer, is not promising.

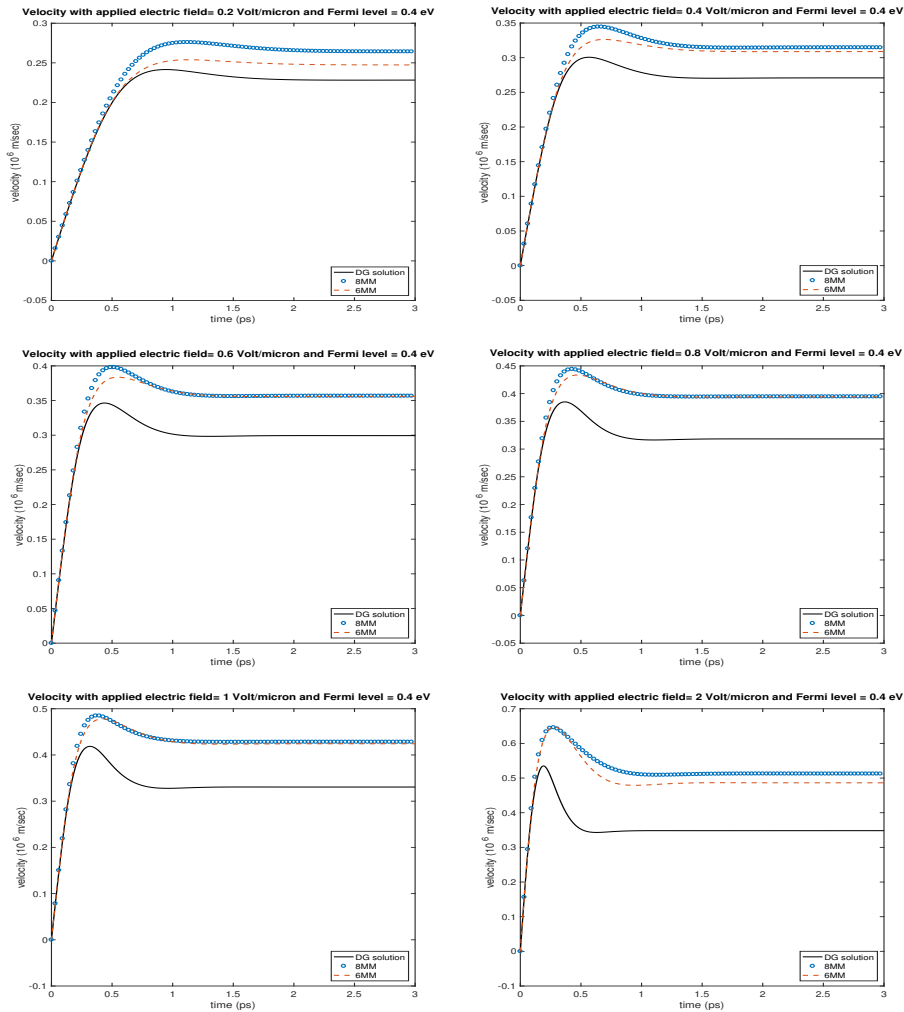


FIGURE 2. Comparison of the average velocity obtained with a direct solution of the Boltzmann equation (DG method) (continuous line), the 8MM hydrodynamical model (circled line) and the 6MM hydrodynamical model (dashed lines) for electric fields  $E = 2$  kV/cm,  $E = 4$  kV/cm,  $E = 6$  kV/cm,  $E = 8$  kV/cm,  $E = 10$  kV/cm,  $E = 20$  kV/cm by considering a constant lattice temperature of 300 K and a Fermi energy equal to 0.4 eV.

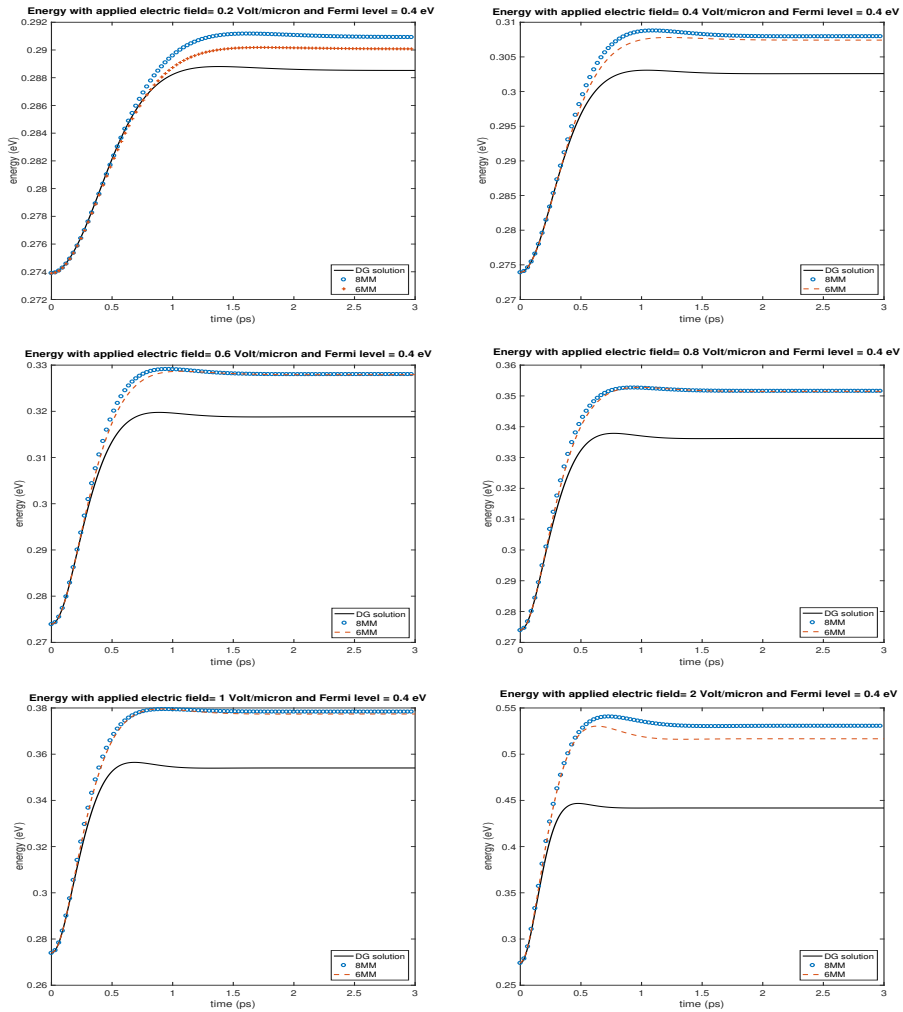


FIGURE 3. Comparison of the average energy obtained with a direct solution of the Boltzmann equation (DG method) (continuous line), the 8MM hydrodynamical model (circled line) and the 6MM hydrodynamical model (dashed lines) for electric fields  $E = 2$  kV/cm,  $E = 4$  kV/cm,  $E = 6$  kV/cm,  $E = 8$  kV/cm,  $E = 10$  kV/cm,  $E = 20$  kV/cm by considering a constant lattice temperature of 300 K and a Fermi energy equal to 0.4 eV.

### 7. Conclusions

A hydrodynamical model for charge transport in graphene has been presented trying to improve the results of Camiola and Romano (2014) with the inclusion of additional moments related to quadratic power of energy. In pristine graphene, the numerical solutions

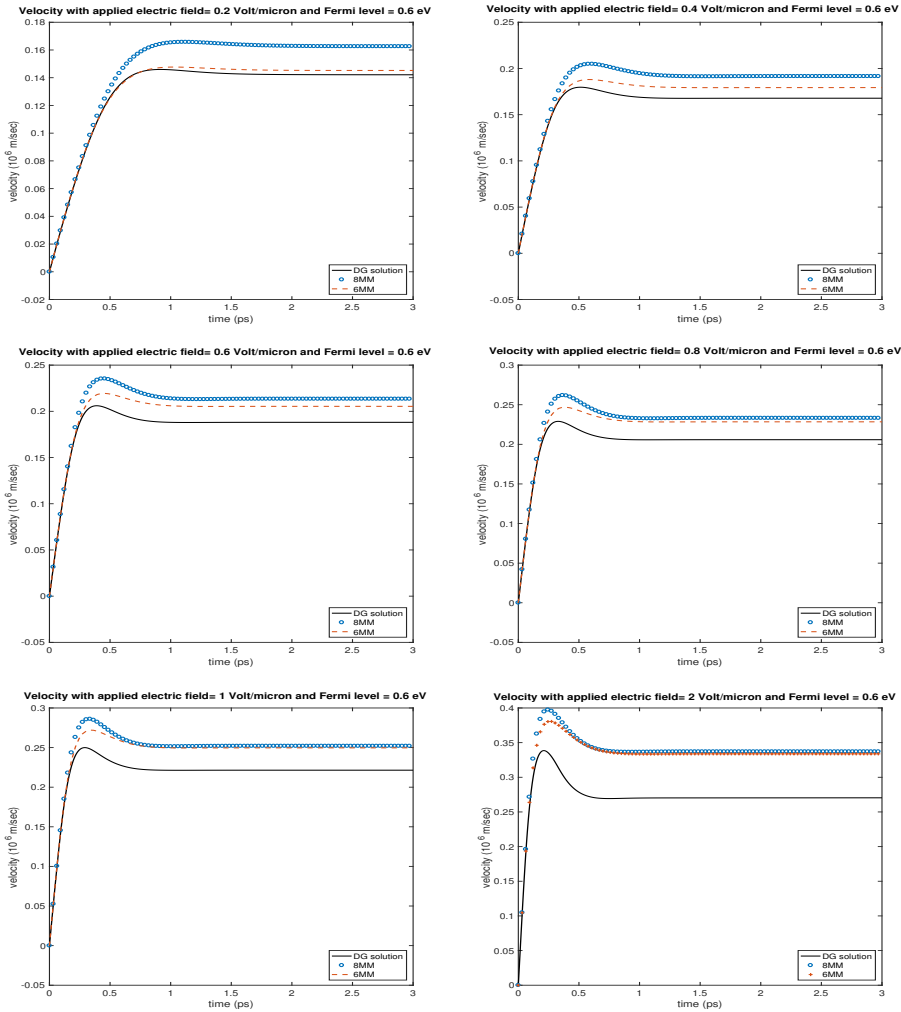


FIGURE 4. Comparison of the average velocity obtained with a direct solution of the Boltzmann equation (DG method) (continuous line), the 8MM hydrodynamical model (circled line) and the 6MM hydrodynamical model (dashed lines) for electric fields  $E = 2$  kV/cm,  $E = 4$  kV/cm,  $E = 6$  kV/cm,  $E = 8$  kV/cm,  $E = 10$  kV/cm,  $E = 20$  kV/cm by considering a constant lattice temperature of 300 K and a Fermi energy equal to 0.6 eV.

given by such a model have been compared with those of the semiclassical Boltzmann equation obtained by a DG method. Apparently no real improvement is achieved with respect to the model of Camiola and Romano (2014). Therefore, the formulation of models more accurate than that of Camiola and Romano (2014) has to be based on a different set of weight function.

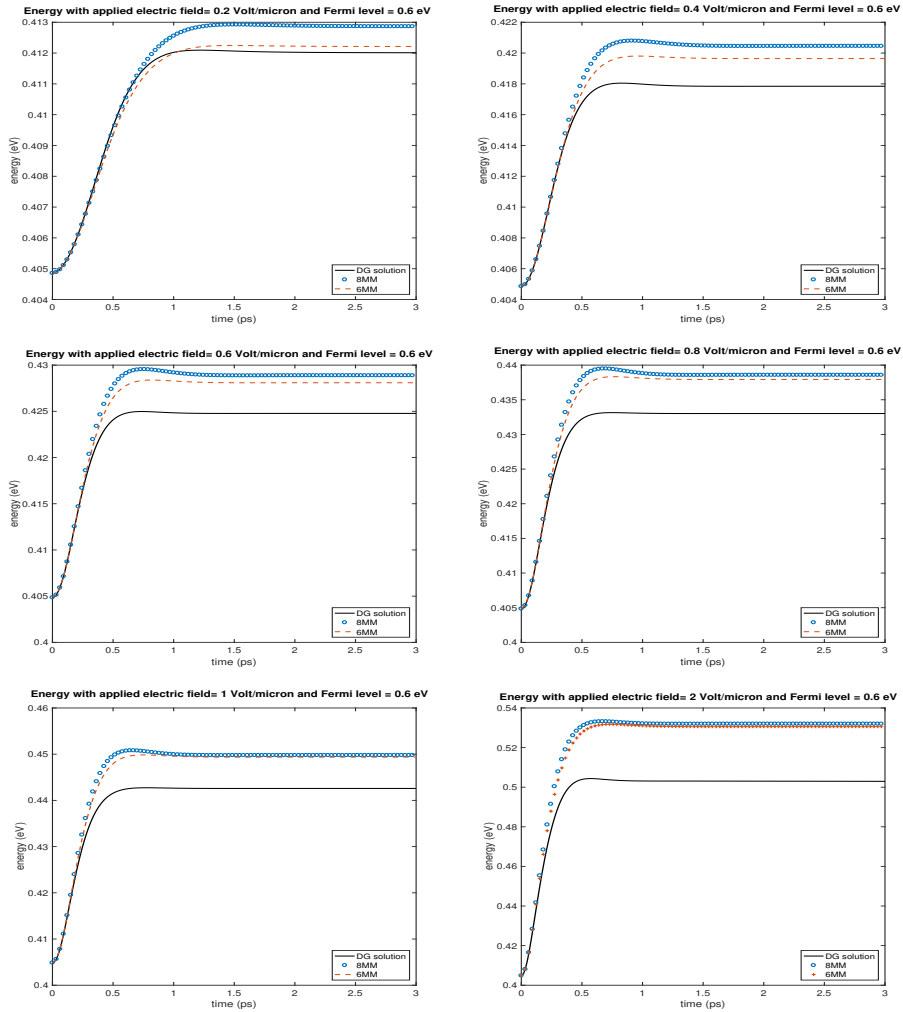


FIGURE 5. Comparison of the average energy obtained with a direct solution of the Boltzmann equation (DG method) (continuous line), the 8MM hydrodynamical model (circled line) and the 6MM hydrodynamical model (dashed lines) for electric fields  $E = 2$  kV/cm,  $E = 4$  kV/cm,  $E = 6$  kV/cm,  $E = 8$  kV/cm,  $E = 10$  kV/cm,  $E = 20$  kV/cm by considering a constant lattice temperature of 300 K and a Fermi energy equal to 0.6 eV.

## Acknowledgments

The authors acknowledge the financial support by INDAM (Istituto Nazionale di Alta Matematica F. Severi).

### ***In Memoriam***

*This paper has been written by one of the author (V.R.) in memory of the friend and colleague Gaetano Giaquinta. V.R. still remembers the pleasant discussions with him at the Engineering Faculty about science, philosophy and art. The author met often Gaetano Giaquinta during the break of their lectures and it was very interesting to hear his point of view about Academia and teaching. V.R. highly missed the wide culture of Gaetano Giaquinta and his in-depth insights on Physics.*

### **References**

- Ali, G., Mascali, G., Romano, V., and Torcasio, R. C. (2012). “A Hydrodynamic Model for Covalent Semiconductors with Applications to GaN and SiC”. *Acta Applicandae Mathematicae*. DOI: [10.1007/s10440-012-9747-6](https://doi.org/10.1007/s10440-012-9747-6).
- Barletti, L. (2014). “Hydrodynamic equations for electrons in graphene obtained from the maximum entropy principle”. *Journal of Mathematical Physics* **55**(8), 083303. DOI: [10.1063/1.4886698](https://doi.org/10.1063/1.4886698).
- Barletti, L. (2016). “Hydrodynamic equations for an electron gas in graphene”. *Journal of Mathematics in Industry* **6**(1). DOI: [10.1186/s13362-016-0023-7](https://doi.org/10.1186/s13362-016-0023-7).
- Borysenko, K. M., Mullen, J. T., Barry, E. A., Paul, S., Semenov, Y. G., Zavada, J. M., Nardelli, M. B., and Kim, K. W. (2010). “First-principles analysis of electron-phonon interactions in graphene”. *Physical Review B* **81**(12). DOI: [10.1103/physrevb.81.121412](https://doi.org/10.1103/physrevb.81.121412).
- Camiola, V. D. and Romano, V. (2014). “Hydrodynamical Model for Charge Transport in Graphene”. *Journal of Statistical Physics* **157**(6), 1114–1137. DOI: [10.1007/s10955-014-1102-z](https://doi.org/10.1007/s10955-014-1102-z).
- Camiola, V. D., Mascali, G., and Romano, V. (2011). “Numerical simulation of a double-gate MOSFET with a subband model for semiconductors based on the maximum entropy principle”. *Continuum Mechanics and Thermodynamics* **24**(4-6), 417–436. DOI: [10.1007/s00161-011-0217-6](https://doi.org/10.1007/s00161-011-0217-6).
- Camiola, V. D., Mascali, G., and Romano, V. (2013). “Simulation of a double-gate MOSFET by a non-parabolic energy-transport subband model for semiconductors based on the maximum entropy principle”. *Mathematical and Computer Modelling* **58**(1-2), 321–343. DOI: [10.1016/j.mcm.2012.11.007](https://doi.org/10.1016/j.mcm.2012.11.007).
- Coco, M., Mascali, G., and Romano, V. (2016a). “Monte Carlo Analysis of Thermal Effects in Monolayer Graphene”. *Journal of Computational and Theoretical Transport* **45**(7), 540–553. DOI: [10.1080/23324309.2016.1211537](https://doi.org/10.1080/23324309.2016.1211537).
- Coco, M., Majorana, A., and Romano, V. (2016b). “Cross validation of discontinuous Galerkin method and Monte Carlo simulations of charge transport in graphene on substrate”. *Ricerche di Matematica* **66**(1), 201–220. DOI: [10.1007/s11587-016-0298-4](https://doi.org/10.1007/s11587-016-0298-4).
- Jaynes, E. T. (1957). “Information Theory and Statistical Mechanics”. *Phys. Rev.* **106**, 620.
- Jou, D. and Lebon, G. (2010). *Extended Irreversible Thermodynamics*. Springer Netherlands. DOI: [10.1007/978-90-481-3074-0](https://doi.org/10.1007/978-90-481-3074-0).
- Lichtenberger, P., Morandi, O., and Schürer, F. (2011). “High-field transport and optical phonon scattering in graphene”. *Physical Review B* **84**(4). DOI: [10.1103/physrevb.84.045406](https://doi.org/10.1103/physrevb.84.045406).
- Majorana, A., Mascali, G., and Romano, V. (2016). “Charge transport and mobility in monolayer graphene”. *Journal of Mathematics in Industry* **7**(1). DOI: [10.1186/s13362-016-0027-3](https://doi.org/10.1186/s13362-016-0027-3).
- Majorana, A. and Romano, V. (2017). “Numerical Solutions of the Spatially Homogeneous Boltzmann Equation for Electrons in n-Doped Graphene on a Substrate”. *Journal of Computational and Theoretical Transport* **46**(3), 176–185. DOI: [10.1080/23324309.2017.1311267](https://doi.org/10.1080/23324309.2017.1311267).
- Mascali, G. and Romano, V. (1997). “Maximum entropy principle in relativistic radiation hydrodynamics”. *Annales de l’I.H.P. Physique théorique* **67**, 123–144.

- Mascali, G. and Romano, V. (2005). “Si and GaAs mobility derived from a hydrodynamical model for semiconductors based on the maximum entropy principle”. *Physica A: Statistical Mechanics and its Applications* **352**(2-4), 459–476. DOI: [10.1016/j.physa.2004.12.058](https://doi.org/10.1016/j.physa.2004.12.058).
- Mascali, G. (2015). “A hydrodynamic model for silicon semiconductors including crystal heating”. *European Journal of Applied Mathematics* **26**(04), 477–496. DOI: [10.1017/s0956792515000157](https://doi.org/10.1017/s0956792515000157).
- Mascali, G. (2016). “A New Formula for Thermal Conductivity Based on a Hierarchy of Hydrodynamical Models”. *Journal of Statistical Physics* **163**(5), 1268–1284. DOI: [10.1007/s10955-016-1509-9](https://doi.org/10.1007/s10955-016-1509-9).
- Mascali, G. and Romano, V. (2011). “A hydrodynamical model for holes in silicon semiconductors: The case of non-parabolic warped bands”. *Mathematical and Computer Modelling* **53**(1-2), 213–229. DOI: [10.1016/j.mcm.2010.08.007](https://doi.org/10.1016/j.mcm.2010.08.007).
- Mascali, G. and Romano, V. (2017a). “Charge Transport in Graphene including Thermal Effects”. *SIAM Journal on Applied Mathematics* **77**(2), 593–613. DOI: [10.1137/15m1052573](https://doi.org/10.1137/15m1052573).
- Mascali, G. and Romano, V. (2017b). “Exploitation of the Maximum Entropy Principle in Mathematical Modeling of Charge Transport in Semiconductors”. *Entropy* **19**(1), 36. DOI: [10.3390/e19010036](https://doi.org/10.3390/e19010036).
- Morandi, O. and Barletti, L. (2014). “Particle Dynamics in Graphene: Collimated Beam Limit”. *Journal of Computational and Theoretical Transport* **43**(1-7), 418–432. DOI: [10.1080/00411450.2014.942917](https://doi.org/10.1080/00411450.2014.942917).
- Morandi, O. and Schürerer, F. (2011). “Wigner model for quantum transport in graphene”. *Journal of Physics A: Mathematical and Theoretical* **44**(26), 265301. DOI: [10.1088/1751-8113/44/26/265301](https://doi.org/10.1088/1751-8113/44/26/265301).
- Müller, I. and Ruggeri, T. (1998). *Rational Extended Thermodynamics*. Springer New York. DOI: [10.1007/978-1-4612-2210-1](https://doi.org/10.1007/978-1-4612-2210-1).
- Muscato, O. and Stefano, V. D. (2013). “Hydrodynamic simulation of a n+ -n+ silicon nanowire”. *Continuum Mechanics and Thermodynamics* **26**(2), 197–205. DOI: [10.1007/s00161-013-0296-7](https://doi.org/10.1007/s00161-013-0296-7).
- Muscato, O. and Wagner, W. (2016). “A Class of Stochastic Algorithms for the Wigner Equation”. *SIAM Journal on Scientific Computing* **38**(3), A1483–A1507. DOI: [10.1137/16m105798x](https://doi.org/10.1137/16m105798x).
- Neto, A. H. C., Guinea, F., Peres, N. M. R., Novoselov, K. S., and Geim, A. K. (2009). “The electronic properties of graphene”. *Reviews of Modern Physics* **81**(1), 109–162. DOI: [10.1103/revmodphys.81.109](https://doi.org/10.1103/revmodphys.81.109).
- Nika, D. L. and Balandin, A. A. (2012). “Two-dimensional phonon transport in graphene”. *Journal of Physics: Condensed Matter* **24**(23), 233203. DOI: [10.1088/0953-8984/24/23/233203](https://doi.org/10.1088/0953-8984/24/23/233203).
- Pop, E., Varshney, V., and Roy, A. K. (2012). “Thermal properties of graphene: Fundamentals and applications”. *MRS Bulletin* **37**(12), 1273–1281. DOI: [10.1557/mrs.2012.203](https://doi.org/10.1557/mrs.2012.203).
- Romano, V. (2007). “Quantum corrections to the semiclassical hydrodynamical model of semiconductors based on the maximum entropy principle”. *Journal of Mathematical Physics* **48**(12), 123504. DOI: [10.1063/1.2819600](https://doi.org/10.1063/1.2819600).
- Romano, V. and Zwierz, M. (2010). “Electron-phonon hydrodynamical model for semiconductors”. *Zeitschrift für angewandte Mathematik und Physik* **61**(6), 1111–1131. DOI: [10.1007/s00033-010-0089-9](https://doi.org/10.1007/s00033-010-0089-9).
- Romano, V. (2002). “2D Simulation of a Silicon MESFET with a Nonparabolic Hydrodynamical Model Based on the Maximum Entropy Principle”. *Journal of Computational Physics* **176**(1), 70–92. DOI: [10.1006/jcph.2001.6968](https://doi.org/10.1006/jcph.2001.6968).
- Romano, V., Majorana, A., and Coco, M. (2015). “DSMC method consistent with the Pauli exclusion principle and comparison with deterministic solutions for charge transport in graphene”. *Journal of Computational Physics* **302**, 267–284. DOI: [10.1016/j.jcp.2015.08.047](https://doi.org/10.1016/j.jcp.2015.08.047).
- Rosa, S. L., Mascali, G., and Romano, V. (2009). “Exact Maximum Entropy Closure of the Hydrodynamical Model for Si Semiconductors: The 8-Moment Case”. *SIAM Journal on Applied Mathematics* **70**(3), 710–734. DOI: [10.1137/080714282](https://doi.org/10.1137/080714282).

- Rosa, S. L. and Romano, V. (2008). “The maximum entropy principle hydrodynamical model for holes in silicon semiconductors: the case of the warped bands”. *Journal of Physics A: Mathematical and Theoretical* **41**(21), 215103. DOI: [10.1088/1751-8113/41/21/215103](https://doi.org/10.1088/1751-8113/41/21/215103).
- Zhao, H., Guo, Q., Xia, F., and Wang, H. (2015). “Two-dimensional materials for nanophotonics application”. *Nanophotonics* **4**(1). DOI: [10.1515/nanoph-2014-0022](https://doi.org/10.1515/nanoph-2014-0022).
- 

<sup>a</sup> Università degli Studi di Catania,  
Dipartimento di Matematica e Informatica,  
Viale Andrea Doria 6, 95125 Catania, Italy.

\* To whom correspondence should be addressed | email: [romano@dmi.unict.it](mailto:romano@dmi.unict.it)

Manuscript received 4 December 2017; published online 13 August 2018

---



© 2018 by the author(s); licensee *Accademia Peloritana dei Pericolanti* (Messina, Italy). This article is an open access article distributed under the terms and conditions of the [Creative Commons Attribution 4.0 International License](https://creativecommons.org/licenses/by/4.0/) (<https://creativecommons.org/licenses/by/4.0/>).