

# Semi-classical and Quantum Hydrodynamic Modeling of Electron Transport in Graphene



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**Abstract** The present work aims at formulating hydrodynamic models for a proper description of charge transport in graphene, which is extremely important for growing technological development in CAD tools. The analysis is carried out in two different steps. Initially a semi-classical hydrodynamic model is developed starting from the moment system associated with Boltzmann equation and obtaining the closure relations with the Maximum Entropy Principle. At this level quantum effects are neglected. In the second step the model previously developed is extended to include quantum effects by incorporating the first order quantum corrections. To assess the validity of this model numerical simulations are under current investigation.

## 1 Introduction

Graphene, a monolayer of  $sp^2$ -bonded carbon atoms with zero band gap, is not only the basis for graphite but also a new material with immense potential in microelectronics for its exceptional electrical transport properties, like high conductivity and high charge mobility. As a result of its promising properties, it seems to be an ideal candidate to take over from silicon for the next generation of faster and smaller electronic devices.

To deal with the basic kinetic transport equations remains too expensive for real life applications. Nevertheless from transport equations it is possible to derive simpler fluid dynamic equations for macroscopic quantities like particle, velocity, or energy densities. They represent a good compromise between physical accuracy and computational cost.

A standard approach to derive macroscopic models, like drift-diffusion, energy transport or hydrodynamic ones, is the moments method. The present work aims at

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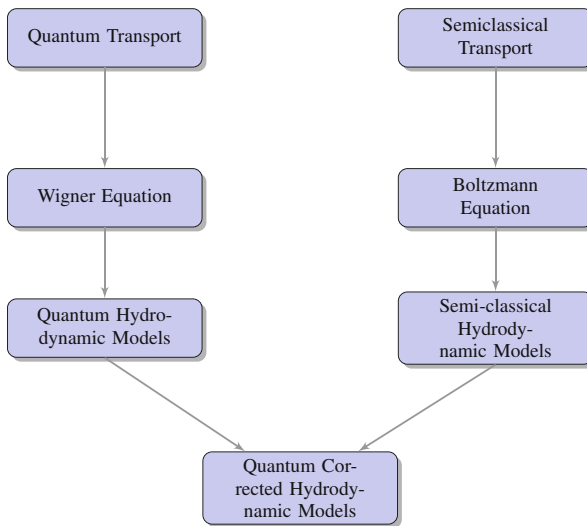
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formulating hydrodynamic models of this type for a proper description of charge transport in graphene, which is extremely important for growing technological development in CAD tools.

The plan of the paper is as follows.

Section 2 focuses on the formulation of a semi-classical hydrodynamic model based on the Maximum Entropy Principle (MEP) without taking into account quantum effects. The model analyzed can be developed by taking into account fully non linear closure relations [11], or its linearized version [2, 12].

To take into account quantum phenomena, in the second section a quantum hydrodynamic model for charge transport in graphene is derived from a moment expansion of the Wigner-Boltzmann equation and the needed closure relations are obtained by adding quantum corrections based on the equilibrium Wigner function to the semiclassical model formulated in [2, 11, 12] by exploiting the Maximum Entropy Principle. The expression of the equilibrium Wigner function which takes into account the energy band of graphene has been obtained by solving the corresponding Bloch equation (see also [1, 17]). In other terms, the strategy adopted for formulating these models combines quantum and semi-classical approaches as shown in Fig. 1.



**Fig. 1** Schematic representation of the strategy adopted for developing Quantum Corrected Hydrodynamic models

## 2 A Semi-classical Hydrodynamic Model

The starting point for the derivation of semi-classical hydrodynamic models is the semi-classical Boltzmann equation

$$\frac{\partial f(\mathbf{r}, \mathbf{k}, t)}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{r}} f(\mathbf{r}, \mathbf{k}, t) + \frac{q}{\hbar} \nabla_{\mathbf{r}} \Phi(\mathbf{r}) \cdot \nabla_{\mathbf{k}} f(\mathbf{r}, \mathbf{k}, t) = \mathcal{C}[f](\mathbf{r}, \mathbf{k}, t) \quad (1)$$

where  $f(\mathbf{r}, \mathbf{k}, t)$  is the distribution of electrons in the conduction or valence band (the dependence from the Dirac point is omitted),  $\nabla_{\mathbf{r}}$  and  $\nabla_{\mathbf{k}}$  are the gradients with respect to the space variable  $\mathbf{r}$  and wave vector respectively,  $q$  is the elementary (positive) charge,  $\hbar$  is the reduced Planck's constant,  $\Phi$  is the electric potential and  $\mathbf{v}$  is the microscopic velocity which is related to the energy band by  $\mathbf{v}(\mathbf{k}) = \pm \frac{1}{\hbar} \nabla_{\mathbf{k}} \mathcal{E}(\mathbf{k})$ . The positive sign refers to the conduction band, the negative sign to the valence one.  $\mathcal{C}$  is the collision term representing the interactions of electrons with acoustic (ac) phonons, longitudinal (*LO*) and transversal (*TO*) optical phonons and *K*-phonons (for more details see [2, 11]).

Numerical solutions of Eq. (1) can be obtained, for example, via Direct Monte Carlo Simulation (DSMC)[5, 22] or by finite difference schemes [10] or by discontinuous Galerkin (DG) methods [5]. However, these simulations have been obtained for simple cases such as pristine graphene under the effect of a constant external electric field. With a view of more complex situations, like those represented by a metal-oxide-semiconductor field-effect transistor (MOSFET) with a graphene channel, it is better to benefit from simpler models like drift-diffusion, energy transport or hydrodynamic ones. These directly provide balance equations for macroscopic quantities like electron density, average velocity or current, average energy, etc., and, therefore, are more suited as models for CAD tools.

The macroscopic quantities are related to the distribution function because they represent average values of some functions of the wave vector  $\mathbf{k}$ . For example, the density  $n(\mathbf{r}, t)$  is given by

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

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

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

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. (1) for  $\psi(\mathbf{k})$  and by integrating with respect to  $\mathbf{k}$

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

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

The main issue related to any model based on balance equations deduced as moment equations of type (2) is that there are more unknowns than introduced moments in the evolution equations, and the so-called *closure problem* arises. This comes from expressing the additional unknowns, that is the extra fluxes and 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 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 [8] (for a general review of the application of MEP to semiconductors the interested reader is referred to [15]). The central idea of this principle is to predict the distribution of the microstates, which are the particle of the system, on the basis of the knowledge of some macroscopic data. The latter information is specified in the form of some simple moment constraints. Therefore the distribution obtained with MEP is the least biased estimator from 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 by solving the following constrained optimization problem: for fixed  $\mathbf{r}$  and  $t$ ,

$$\begin{aligned} \max_{f \in \mathcal{F}} S[f] \quad \text{subject to the constraints:} \\ 0 < f < 1, \end{aligned} \quad (3)$$

$$M_A = \frac{2}{(2\pi)^2} \int_{\mathbb{R}^2} \psi_A(\mathbf{k}) f(\mathbf{r}, \mathbf{k}, t) d^2\mathbf{k}, \quad A = 1, 2, \dots, N, \quad (4)$$

where  $S[f]$  is the entropy of the system, which in the semi-classical approximation reads

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

Factor 2 is included to take into account the valley degeneracy.  $\mathcal{F}$  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  $\mathbb{R}^2$ .

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

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

Let the variation of  $S'$  with respect to  $f$  be zero, i.e.,

$$0 = \delta S' = -2 \frac{2k_B}{(2\pi)^2} \int_{\mathbb{R}^2} \left[ \ln f - \ln(1-f) + \frac{1}{2k_B} \sum_A \psi_A(\mathbf{k}) \lambda_A \right] \delta f d^2 \mathbf{k}.$$

Since  $\delta f$  is arbitrary, the quantity in the square brackets must be zero; we get

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

which also fulfills the unilateral constraints (3).

The multiplicative constant  $\frac{1}{2k_B}$  has been included into the multipliers for simplicity.

To complete the optimization procedure, it is necessary to invert the relations (4) and express the Lagrangian multipliers as functions of the basic variables. This can generally be achieved only numerically or by some approximation, e.g. expanding around the equilibrium state.

The above problem of inversion apart, once one gets  $f_{MEP}$ , the needed closure relations are obtained by evaluating the extra fluxes and production terms with  $f_{MEP}$  instead of  $f$ . At equilibrium the distribution of electrons, both in the conduction and valence band, are given by the Fermi-Dirac distribution

$$f_{FD}(\mathbf{r}, \mathbf{k}, t) = \frac{1}{1 + \exp \left( \frac{\mathcal{E}(\mathbf{k}) - \varepsilon_F}{k_B T_L} \right)}, \quad -\infty < \mathcal{E}(\mathbf{k}) < +\infty, \quad (5)$$

where  $\varepsilon_F$  is the Fermi energy,  $T_L$  being the lattice temperature and  $k_B$  the Boltzmann constant.

In this work we consider a 6-moment model obtained by choosing as weight functions  $\{1, \mathcal{E}, \mathbf{v}, \mathcal{E}\mathbf{v}\}$  to which the following average quantities in the conduction bands (similar results hold for the valence band) correspond

$$n(\mathbf{r}, t) = \frac{2}{(2\pi)^2} \int_{\mathbb{R}^2} f(\mathbf{r}, \mathbf{k}, t) d\mathbf{k} \quad \text{density,} \quad (6)$$

$$n(\mathbf{r}, t)W(\mathbf{r}, t) = \frac{2}{(2\pi)^2} \int_{\mathbb{R}^2} f(\mathbf{r}, \mathbf{k}, t)\mathcal{E}(\mathbf{k}) d\mathbf{k} \quad \text{energy density,} \quad (7)$$

$$n(\mathbf{r}, t)\mathbf{V}(\mathbf{r}, t) = \frac{2}{(2\pi)^2} \int_{\mathbb{R}^2} f(\mathbf{r}, \mathbf{k}, t)\mathbf{v}(\mathbf{k}) d\mathbf{k} \quad \text{linear momentum density,} \quad (8)$$

$$n(\mathbf{r}, t)\mathbf{S}(\mathbf{r}, t) = \frac{2}{(2\pi)^2} \int_{\mathbb{R}^2} f(\mathbf{r}, \mathbf{k}, t)\mathcal{E}(\mathbf{k})\mathbf{v}(\mathbf{k}) d\mathbf{k} \quad \text{energy-flux density.} \quad (9)$$

The corresponding evolution equations, in the unipolar case, are given by

$$\begin{aligned} \frac{\partial}{\partial t} n + \nabla_{\mathbf{r}} (n \mathbf{V}) &= 0, \\ \frac{\partial}{\partial t} (n W) + \nabla_{\mathbf{r}} (n \mathbf{S}) + q n \mathbf{E} \cdot \mathbf{V} &= n C_W, \\ \frac{\partial}{\partial t} (n \mathbf{V}) + \nabla_{\mathbf{r}} (n \mathbf{F}^{(0)}) + q n \mathbf{G}^{(0)} : \mathbf{E} &= n C_{\mathbf{V}}, \\ \frac{\partial}{\partial t} (n \mathbf{S}) + \nabla_{\mathbf{r}} (n \mathbf{F}^{(1)}) + q n \mathbf{G}^{(1)} : \mathbf{E} &= n C_{\mathbf{S}}. \end{aligned}$$

Besides the average densities, velocities, energies and energy fluxes, additional quantities appear<sup>1</sup>

$$\begin{aligned} n C_{\mathbf{V}} &= \frac{2}{(2\pi)^2} \int_{\mathbb{R}^2} \mathbf{v}(\mathbf{k}) \mathcal{C}(\mathbf{k}) d\mathbf{k}, \\ n C_W &= \frac{2}{(2\pi)^2} \int_{\mathbb{R}^2} \mathcal{E}(\mathbf{k}) \mathcal{C}(\mathbf{k}) d\mathbf{k}, \quad n C_{\mathbf{S}} = \frac{2}{(2\pi)^2} \int_{\mathbb{R}^2} \mathcal{E}(\mathbf{k}) \mathbf{v}(\mathbf{k}) \mathcal{C}(\mathbf{k}) d\mathbf{k} \\ n \begin{pmatrix} \mathbf{F}^{(0)} \\ \mathbf{F}^{(1)} \end{pmatrix} &= \frac{2}{(2\pi)^2} \int_{\mathbb{R}^2} \begin{pmatrix} 1 \\ \mathcal{E}(\mathbf{k}) \end{pmatrix} \mathbf{v}(\mathbf{k}) \otimes \mathbf{v}(\mathbf{k}) f(\mathbf{r}, \mathbf{k}, t) d\mathbf{k}, \\ n \begin{pmatrix} \mathbf{G}^{(0)} \\ \mathbf{G}^{(1)} \end{pmatrix} &= \frac{2}{\hbar (2\pi)^2} \int_{\mathbb{R}^2} f(\mathbf{r}, \mathbf{k}, t) \nabla_{\mathbf{k}} \begin{pmatrix} \mathbf{v}(\mathbf{k}) \\ \mathcal{E}(\mathbf{k}) \mathbf{v}(\mathbf{k}) \end{pmatrix} d\mathbf{k}, \end{aligned}$$

that must be expressed as function of the basic variables  $n, \mathbf{V}, W, \mathbf{S}$ .

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

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

$$C_M = C_M^{(ac)} + \sum_{s=L,O,T,O,K} C_M^{(s)},$$

with  $M = \rho, W, \mathbf{V}, \mathbf{S}$ .

The following expression of the distribution function deduced by MEP

$$f_{MEP}(\mathbf{r}, \mathbf{k}, t) = \frac{1}{1 + \exp(\lambda(\mathbf{r}, t) + \lambda_w(\mathbf{r}, t)\mathcal{E}(\mathbf{k}) + (\lambda_{\mathbf{V}}(\mathbf{r}, t) + \mathcal{E}(\mathbf{k})\lambda_{\mathbf{S}}(\mathbf{r}, t)) \cdot \mathbf{v}(\mathbf{k}))} \quad (10)$$

has been used in the linearized form<sup>2</sup>

$$f_{MEP}(\mathbf{r}, \mathbf{k}, t) \approx \frac{1}{1 + e^{\lambda + \lambda_w \mathcal{E}}} - \frac{e^{\lambda + \lambda_w \mathcal{E}}}{(1 + e^{\lambda + \lambda_w \mathcal{E}})^2} (\lambda_{\mathbf{V}} + \mathcal{E} \lambda_{\mathbf{S}}) \cdot \mathbf{v}. \quad (11)$$

Explicit closure relation has been obtained in [2] and [16] the crystal heating effects have been also included. Comparisons with Direct Simulation Monte Carlo [4–6, 13, 14, 22] have shown a good accuracy of the model. In the next section the general guideline for getting quantum corrections to the semiclassical hydrodynamic models will be delineated.

### 3 A 6-Moment Model with Quantum Corrections

To take into account quantum phenomena, the semiclassical Boltzmann equation is not enough to describe charge transport. As a starting point for deriving the quantum corrections to the semiclassical model, we consider the Wigner equation. At zero order we recover the semiclassical models developed in [2, 11, 12, 16] by exploiting the Maximum Entropy Principle (MEP). By following the idea developed in [20] for silicon,  $\hbar^2$  order corrections are obtained from the scaling of high field and collision dominated regime. In the limit of high collisional frequency of the quantum correction to the collision operator, this is equivalent to determine the  $\hbar^2$  order corrections with the equilibrium Wigner function, similarly to what done in [7]. The problem to find out the equilibrium Wigner function in the case of an arbitrary energy band has been discussed in [21] where the corresponding Bloch equation is written and solved for silicon in the Kane dispersion relation approximation. Here the same approach is used for graphene.

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

One important issue is related to the conical shape of the energy band around the Dirac points of the first Brillouin zone. This fact makes singular some term of the expansion if a sharp zero gap between the conduction and the valence band is assumed. However, see for example [3], from a theoretical point of view it is possible the presence, although very small, of a gap which is related to the first and second neighbour hopping energy. Therefore, around the Dirac points we employ a regularized energy band. Explicit formulas are obtained and the resulting model is given by a set of dispersive PDEs.

Of course it is also possible to try to numerically solve directly the Wigner equation but major computational difficulties arise and at the present time it seems far from being a standard feasible tool for the design of electron devices. The interested reader can see the monograph [19] and the paper [5, 18, 22] for recent advances of the algorithms in stochastic approaches.

### 3.1 Wigner Equation

In the proximity of the Dirac points  $K$  ( $K'$ ), which are the vertices of the Brillouin zone, by choosing in the  $\mathbf{k}$ -space a reference frame centered in the considered Dirac point, the energy dispersion relation can be considered approximately linear with respect to the modulus of the wave-vector  $\mathbf{k}$ . As already mentioned above it is not clear if a small gap between the conduction and the valence band exists. Therefore we adopt the following regularization

$$\mathcal{E}(\mathbf{k}) = \pm v_F \sqrt{a^2 + p^2},$$

where  $p = \hbar|\mathbf{k}|$ ,  $v_F \simeq 1 \times 10^6$  cm/s is the Fermi velocity,  $\hbar$  is the reduced Planck's constant. The sign “+” refers to the conduction band while the sign “-” refers to the valence band.  $a$  is a small parameter related to the nearest-neighbour hopping energy [3]. To derive a transport equation, we introduce the single electron Wigner quasi-distribution  $w(\mathbf{x}, p, t)$ , depending on the position  $\mathbf{x}$ , momentum  $p$  and time  $t$ . Evolution is governed by the *Wigner-Poisson* system for  $w$  and the electrostatic potential  $\Phi$

$$\frac{\partial w(\mathbf{x}, p, t)}{\partial t} + S[\mathcal{E}]w(\mathbf{x}, p, t) - q\theta[\mathcal{E}]w(\mathbf{x}, p, t) = C[w],$$

$$\nabla \cdot (\epsilon \nabla \Phi) = -q(N_D - n),$$

where  $q$  is the elementary (positive) charge,  $N_D$  is donor carrier concentration,  $C[w]$  is the collision term representing the electron-phonon scattering while  $S[\mathcal{E}]$  and  $\theta[\mathcal{E}]$



represent the pseudo-differential operators

$$S[\mathcal{E}]w(\mathbf{x}, p, t) = \frac{i}{\hbar(2\pi)^2} \int_{\mathbb{R}_{\mathbf{x}'}^2 \times \mathbb{R}_{\mathbf{v}}^2} [\mathcal{E}(p + \frac{\hbar}{2}\mathbf{v}, t) + \\ - \mathcal{E}(p - \frac{\hbar}{2}\mathbf{v}, t)]w(\mathbf{x}', p, t)e^{-i(\mathbf{x}' - \mathbf{x}) \cdot \mathbf{v}} d\mathbf{x}' d\mathbf{v},$$

$$\theta[\mathcal{E}]w(\mathbf{x}, p, t) = \frac{i}{\hbar(2\pi)^2} \int_{\mathbb{R}_{p'}^2 \times \mathbb{R}_{\eta}^2} [\Phi(\mathbf{x} + \frac{\hbar}{2}\boldsymbol{\eta}, t) + \\ - \Phi(\mathbf{x} - \frac{\hbar}{2}\boldsymbol{\eta}, t)]w(\mathbf{x}, p', t)e^{i(p' - p) \cdot \boldsymbol{\eta}} dp' d\boldsymbol{\eta}.$$

In the semiclassical limit  $\hbar \rightarrow 0$ , the Wigner equation reduces to Boltzmann one.

### 3.2 Equilibrium Wigner Function

If we denote the density matrix at equilibrium by  $\rho_{eq}(\mathbf{r}, \mathbf{s}, \beta)$ , it satisfies the Bloch equation

$$\frac{\partial \rho_{eq}(\mathbf{r}, \mathbf{s}, \beta)}{\partial \beta} = -\frac{1}{2}[H_{\mathbf{r}}\rho_{eq}(\mathbf{r}, \mathbf{s}, \beta) + H_{\mathbf{s}}\rho_{eq}(\mathbf{r}, \mathbf{s}, \beta)].$$

Applying the Fourier transform to the Bloch equation, we get

$$\frac{\partial w_{eq}(\mathbf{x}, \mathbf{p}, \beta)}{\partial \beta} = -\frac{1}{2} \left\{ \frac{1}{(2\pi)^2} \int_{\mathbb{R}_{\mathbf{x}'}^2 \times \mathbb{R}_{\mathbf{v}}^2} \mathcal{E} \left( \mathbf{p} + \frac{\hbar}{2}\mathbf{v} \right) + \right. \\ \left. + \mathcal{E} \left( \mathbf{p} - \frac{\hbar}{2}\mathbf{v} \right) w_{eq}(\mathbf{x}', \mathbf{p}, \beta) e^{-i(\mathbf{x}' - \mathbf{x}) \cdot \mathbf{v}} d\mathbf{x}' d\mathbf{v} - \right. \\ \left. - \frac{q}{(2\pi)^2} \int_{\mathbb{R}_{\mathbf{p}'}^2 \times \mathbb{R}_{\boldsymbol{\eta}}^2} \Phi \left( \mathbf{x} + \frac{\hbar}{2}\boldsymbol{\eta} \right) + \Phi \left( \mathbf{x} - \frac{\hbar}{2}\boldsymbol{\eta} \right) w_{eq}(\mathbf{x}, \mathbf{p}', \beta) e^{i(\mathbf{p}' - \mathbf{p}) \cdot \boldsymbol{\eta}} d\mathbf{p}' d\boldsymbol{\eta} \right\},$$

where  $w_{eq}(\mathbf{x}, \mathbf{p}, \beta)$  is the equilibrium Wigner function. We looked for solution of the type

$$w_{eq}(\mathbf{x}, \mathbf{p}, \beta) = w_{eq}^{(0)}(\mathbf{x}, \mathbf{p}, \beta) + \hbar^2 w_{eq}^{(1)}(\mathbf{x}, \mathbf{p}, \beta).$$

After some algebra we get the equilibrium Wigner function

$$w_{eq}(\mathbf{x}, p, \beta) = \exp(q\Phi(\mathbf{x})\beta) \exp(-\beta\mathcal{E}(p)) \left\{ 1 + \frac{q\beta^2\hbar^2}{8} \frac{\partial^2\mathcal{E}(p)}{\partial p_i\partial p_j} \frac{\partial^2\Phi(\mathbf{x})}{\partial x_i\partial x_j} + \right. \\ \left. + \frac{\beta^3\hbar^2}{24} \left[ q^2 \frac{\partial^2\mathcal{E}(p)}{\partial p_i\partial p_j} \frac{\partial\Phi(\mathbf{x})}{\partial x_i} \frac{\partial\Phi(\mathbf{x})}{\partial x_j} - q \frac{\partial^2\Phi(\mathbf{x})}{\partial x_i\partial x_j} v_i v_j \right] \right\} + o(\hbar^2).$$

### 3.3 Structure of the Model

Supposing the expansion

$$w = w^{(0)} + \hbar^2 w^{(1)} + O(\hbar^4)$$

holds and by proceeding formally, as  $\hbar \rightarrow 0$  the Wigner equation gives the semiclassical Boltzmann equation. Therefore we identify  $w^{(0)}(\mathbf{x}, p, t)$  with the semiclassical distribution which has been approximated in [11, 12] with the maximum entropy principle estimator  $w^{(0)}(\mathbf{x}, p, t) \approx f_{MEP}(\mathbf{x}, p, t)$ .

At first order in  $\hbar^2$  one finds

$$\frac{\partial w^{(1)}(\mathbf{x}, p, t)}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{x}} w^{(1)}(\mathbf{x}, p, t) - \frac{1}{24} \frac{\partial^3\mathcal{E}(p)}{\partial p_i\partial p_j\partial p_k} \frac{\partial^3 w^{(0)}(\mathbf{x}, p, t)}{\partial x_i\partial x_j\partial x_k} + \\ + q \nabla_{\mathbf{x}}\Phi(\mathbf{x}) \nabla_p w^{(1)}(\mathbf{x}, p, t) - \frac{q}{24} \frac{\partial^3\Phi(\mathbf{x})}{\partial x_i\partial x_j\partial x_k} \frac{\partial^3 w^{(0)}(\mathbf{x}, p, t)}{\partial p_i\partial p_j\partial p_k} = \mathcal{C}[w^{(1)}]$$

Hereafter, suppose  $w^{(1)} = w_{eq}^{(1)}$ .

As an example, consider a 6-Moment Model based on the following moments

$$\frac{2}{(2\pi\hbar)^2} \int_{\mathbb{R}^2} w(\mathbf{x}, p, t) dp = n(\mathbf{x}, t) \quad \text{density,} \\ \frac{2}{(2\pi\hbar)^2} \int_{\mathbb{R}^2} w(\mathbf{x}, p, t) \mathcal{E}(p) dp = n(\mathbf{x}, t) W \quad \text{energy density,} \\ \frac{2}{(2\pi\hbar)^2} \int_{\mathbb{R}^2} w(\mathbf{x}, p, t) \mathbf{v}(p) dp = n(\mathbf{x}, t) \mathbf{V} \quad \text{linear momentum density,} \\ \frac{2}{(2\pi\hbar)^2} \int_{\mathbb{R}^2} w(\mathbf{x}, p, t) \mathcal{E}(p) \mathbf{v}(p) dp = n(\mathbf{x}, t) \mathbf{S} \quad \text{energy-flux density.}$$

The corresponding evolution equations are given by<sup>3</sup>

$$\frac{\partial}{\partial t} n(\mathbf{x}, t) + \frac{\partial}{\partial x_i} \left( n(\mathbf{x}, t) V_i - \frac{\hbar^2}{24} \frac{\partial^2 (n(\mathbf{x}, t) T_{ijk}^{(0)})}{\partial x_j \partial x_k} \right) = 0, \quad (12)$$

$$\begin{aligned} & \frac{\partial}{\partial t} (n(\mathbf{x}, t) W) + \frac{\partial}{\partial x_i} \left( n(\mathbf{x}, t) S_i - \frac{\hbar^2}{24} \frac{\partial^2 (n(\mathbf{x}, t) T_{ijk}^{(1)})}{\partial x_j \partial x_k} \right) - \\ & - q \frac{\partial}{\partial x_i} \Phi(\mathbf{x}) \cdot n(\mathbf{x}, t) V_i + \frac{q \hbar^2}{24} \frac{\partial^3 \Phi(\mathbf{x})}{\partial x_i \partial x_j \partial x_k} n(\mathbf{x}, t) T_{ijk}^{(0)} = C_W[w^{(0)}], \end{aligned} \quad (13)$$

$$\begin{aligned} & \frac{\partial}{\partial t} (n(\mathbf{x}, t) V_i) + \frac{\partial}{\partial x_j} \left( n(\mathbf{x}, t) F_{ij}^{(0)} - \frac{\hbar^2}{24} \frac{\partial^2 (n(\mathbf{x}, t) H_{ijkl}^{(0)})}{\partial x_k \partial x_l} \right) - \\ & - q \frac{\partial}{\partial x_j} \Phi(\mathbf{x}) \cdot n(\mathbf{x}, t) G_{ij}^{(0)} + \frac{q \hbar^2}{24} \frac{\partial^3 \Phi(\mathbf{x})}{\partial x_j \partial x_k \partial x_l} n(\mathbf{x}, t) L_{ijkl}^{(0)} = C_{V_i}[w^{(0)}], \end{aligned} \quad (14)$$

$$\begin{aligned} & \frac{\partial}{\partial t} (n(\mathbf{x}, t) S_i) + \frac{\partial}{\partial x_j} \left( n(\mathbf{x}, t) F_{ij}^{(1)} - \frac{\hbar^2}{24} \frac{\partial^2 (n(\mathbf{x}, t) H_{ijkl}^{(1)})}{\partial x_k \partial x_l} \right) - \\ & - q \frac{\partial}{\partial x_j} \Phi(\mathbf{x}) \cdot n(\mathbf{x}, t) V_j \cdot n(\mathbf{x}, t) G_{ij}^{(1)} + \frac{q \hbar^2}{24} \frac{\partial^3 \Phi(\mathbf{x})}{\partial x_j \partial x_k \partial x_l} n(\mathbf{x}, t) L_{ijkl}^{(1)} = C_{S_i}[w^{(0)}] \end{aligned} \quad (15)$$

where  $V_i$  and  $S_i$  are the significant components of macroscopic velocity  $\mathbf{V}$  and energy-flux  $\mathbf{S}$  respectively.

Besides the average densities, velocities, energies and energy fluxes, additional quantities appear

$$\begin{aligned} n(\mathbf{x}, t) \begin{pmatrix} T_{ijk}^{(0)} \\ T_{ijk}^{(1)} \end{pmatrix} &= \frac{2}{(2\pi\hbar)^2} \int_{\mathbb{R}^2} \begin{pmatrix} 1 \\ \mathcal{E}(p) \end{pmatrix} w^{(0)}(\mathbf{x}, p, t) \frac{\partial^3 \mathcal{E}(p)}{\partial p_i \partial p_j \partial p_k} dp, \\ n(\mathbf{x}, t) \begin{pmatrix} H_{ijkl}^{(0)} \\ H_{ijkl}^{(1)} \end{pmatrix} &= \frac{2}{(2\pi\hbar)^2} \int_{\mathbb{R}^2} \begin{pmatrix} 1 \\ \mathcal{E}(p) \end{pmatrix} w^{(0)}(\mathbf{x}, p, t) \frac{\partial^3 \mathcal{E}(p)}{\partial p_i \partial p_j \partial p_k} v_l dp, \\ n(\mathbf{x}, t) \begin{pmatrix} G_{ij}^{(0)} \\ G_{ij}^{(1)} \end{pmatrix} &= \frac{2}{(2\pi\hbar)^2} \int_{\mathbb{R}^2} \begin{pmatrix} 1 \\ \mathcal{E}(p) \end{pmatrix} w(\mathbf{x}, p, t) \frac{\partial^2 \mathcal{E}(p)}{\partial p_i \partial p_j} dp, \\ n(\mathbf{x}, t) \begin{pmatrix} L_{ijkl}^{(0)} \\ L_{ijkl}^{(1)} \end{pmatrix} &= \frac{2}{(2\pi\hbar)^2} \int_{\mathbb{R}^2} \begin{pmatrix} 1 \\ \mathcal{E}(p) \end{pmatrix} w^{(0)}(\mathbf{x}, p, t) \frac{\partial^4 \mathcal{E}(p)}{\partial p_i \partial p_j \partial p_k \partial p_l} dp, \end{aligned}$$

<sup>3</sup>Einstein's summation convention is used.

$$n(\mathbf{x}, t) \begin{pmatrix} F_{ij}^{(0)} \\ F_{ij}^{(1)} \end{pmatrix} = \frac{2}{(2\pi\hbar)^2} \int_{\mathbb{R}^2} \begin{pmatrix} 1 \\ \mathcal{E}(p) \end{pmatrix} w(\mathbf{x}, p, t) v_i v_j dp.$$

that must be expressed as function of the basic variables  $n$ ,  $W$ ,  $\mathbf{V}$ ,  $\mathbf{S}$ . Regarding the production terms, they are given by the sum of contributions arising from the different types of phonon scattering. Explicit closure relations have been obtained and numerical simulations are under current investigation.

## 4 Conclusions and Future Work

Initially a semi-classical hydrodynamic model for charge transport in graphene has been presented. To include quantum effects, the proposed model has been extended by incorporating the first quantum corrections. Therefore in the last section an example of quantum hydrodynamic model for charge transport in graphene has been formulated. It is composed of the semiclassical model presented in [2, 11, 12] augmented with quantum corrections at  $\hbar^2$  order deduced by exploiting the equilibrium Wigner function obtained by solving the Bloch equation in the case of graphene. As  $\hbar \mapsto 0$ , the proposed model of course reduces to the semiclassical one which turned out to be accurate enough when comparison with DSMC results have been performed [11, 12]. Several strategies can be found in the literature for devising quantum hydrodynamic models (the interested reader is referred to [9] for a comprehensive review) but usually strong approximations on the collision terms or on the energy bands are introduced and the semiclassical limit leads to semiclassical models whose soundness is questionable. To assess the validity of the proposed model numerical simulations are under current investigation and they will be presented in a forthcoming article.

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