
TESI DI DOTTORATO

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Modeling and simulation of charge transport in graphene

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Modeling and simulation of charge transport in graphene

TESI DI DOTTORATO

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XXXII CICLO

“Pure mathematics and physics are becoming ever more closely connected, though their methods remain different. One may describe the situation by saying that the mathematician plays a game in which he himself invents the rules while the physicist plays a game in which the rules are provided by Nature, but as time goes on it becomes increasingly evident that the rules which the mathematician finds interesting are the same as those which Nature has chosen”¹.

Paul Adrien Maurice Dirac

¹P.A.M. Dirac. “The Relation between Mathematics and Physics”. In: *Proceedings of the Royal Society of Edinburgh*, 59 (1940), pp. 122–129. doi:10.1017/S0370164600012207

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Introduction

During the last years, there has been a growing interest towards low dimensional materials, and considerable effort has been made to succeed in the ambitious goal of reducing the size of new electronic devices. Graphene has peculiar physical properties that make it one of the most prominent and widely studied low dimensional materials. It was experimentally isolated in 2004 by A. K. Geim and K. S. Novoselov who, for that discovering [38], have been awarded with the Nobel prize in 2010. Graphene has been the object of intense theoretical and experimental research. About its properties [50, 19] we mention that a graphene layer is the thinnest object ever obtained, this material is also the strongest one, it is very elastic and impermeable to any molecule, it is extremely electrically and thermally conductive, charge carriers moves inside it as massless Dirac fermions. The latter makes graphene a wonderful laboratory to study relativistic properties in a classical framework. Moreover, exceptional quantum phenomena were predicted and experimental demonstrated in graphene, e.g, Klein paradox [51, 108] and Veselago lensing [20, 54]. Because of its extraordinary features, graphene is considered to potentially be the revolutionary new material in future development of nano-electronic [19] and optoelectronic devices [109].

We will focus on the electronic properties of graphene. In this framework several studies have been done [7, 56, 73]. We will introduce new results on mathematical modeling and numerical simulation of charge transport. One of the most accurate model for charge transport in graphene is represented by the semiclassical Boltzmann equations for electrons, in the conduction band, and for holes, in the valence band. These Boltzmann equations are coupled through the collision terms, and include several physical effects, such as scatterings between electrons and phonons, between electrons and impurities in the presence of a substrate and between electrons themselves. A new Direct Simulation Monte Carlo (DSMC) method, where the Pauli exclusion principle is correctly included, has been successfully developed in the unipolar space homogeneous case for suspended graphene [89] and for graphene on substrate [25]. In both cases comparisons with numerical solution obtained by a discontinuous Galerkin (DG) approach have addressed the accuracy of the proposed DSMC. To include thermal effects, Boltzmann equations for the phonon dynamic have been also taken into account in [26, 30]. The numerical solutions of the models mentioned above require a high computational effort. Therefore, macroscopic models have been formulated, e.g.,

drift-diffusion, energy-transport or hydrodynamical. For graphene a hydrodynamical model based on the maximum entropy principle (MEP) has been formulated in [18, 58, 59] using a set of field variables which proved to be successful for traditional semiconductors as silicon [69, 88, 87, 92, 91, 76, 66], gallium arsenide [69, 68], silicon carbide [2].

All the above cited papers refer to the space homogeneous case, however industrial applications require solutions in non homogeneous cases. Among electronic devices, Metal Oxide Semiconductor Field Effect Transistor (MOSFET) is the backbone of the modern integrated circuits. For the case in which the active area is made of traditional materials like, for example, silicon or gallium arsenide, a lot of analysis and simulations have been performed in order to optimize the design. Lately, graphene is getting a great attention on account of its peculiar features and, in particular, from the point of view of nano-electronics, for the high electrical conductivity. It is highly tempting trying to replace the traditional semiconductors with graphene in the active area of electronic devices such as the MOSFETs. The main reason is that industry requires smaller and smaller components for advanced integrated circuits. A Field Effect Transistor (FET) having the active area made of graphene is called Graphene Field Effect Transistor (GFET). In the hierarchy of electronic devices modeling the ground level is represented by the drift-diffusion equations, usually coupled with a Poisson equation for the electric potential. The mobility expressions are essential for the drift-diffusion equations to correctly predict the amount of current flowing through the device. A mobility model for highly doped monolayer graphene has been presented in [62], where the fitting curves have been obtained through numerical solutions of the semiclassical Boltzmann equation.

In this thesis we present original results extending the models introduced above. In particular, to quantify the inter-band effects, numerical solutions for the semiclassical Boltzmann equations in the homogeneous and suspended low doped case, have been published in the paper: A. Majorana, G. Nastasi, and V. Romano, "Simulation of Bipolar Charge Transport in Graphene by Using a Discontinuous Galerkin Method", *Commun. Comput. Phys.* 26.1 (2019), pp. 114–134.

The simulations have also been extended to the case of graphene on substrate and presented in the paper: M. Coco and G. Nastasi, "Simulation of bipolar charge transport in graphene on h-BN", *COMPEL* (2020), doi: 10.1108/COMPEL-08-2019-0311. Moreover a comparison in terms of current flow efficiency by means of DSMC can be found in M. Coco, A. Majorana, G. Nastasi, and V. Romano, "High-field mobility in graphene on substrate with a proper inclusion of the Pauli exclusion principle", *Atti Accad. Pelorit. Pericol. Cl. Sci. Fis. Mat. Nat.* 97.S1 (2019), A6.

An enhancement of the mobility model in [62] which includes the bipolar transport,

has been presented in: G. Nastasi and V. Romano, “Improved mobility models for charge transport in graphene”, *Commun. Appl. Ind. Math.* 10.1 (2019), pp. 41–52.

Concerning the development of a drift-diffusion model for GFET, numerical simulations based on finite difference schemes adopting the mobility model of [33] have been obtained in G. Nastasi and V. Romano, “Simulation of graphene field effect transistors”, *Proceedings of SCEE 2018, Mathematics in Industry*, Springer (in press). A further improvement based on the mobility model of [81] have been proposed in the submitted paper: G. Nastasi and V. Romano, “A full coupled drift-diffusion-Poisson simulation of a GFET”.

Part of this thesis has been written during some research stay in other institutions. A first topic, regarding the classical-quantum drift diffusion model of charge transport in graphene, has been investigated during two visiting periods at the Institut de Mathématiques de Toulouse, Université Toulouse III - Paul Sabatier, under the supervision of Prof. C. Negulescu, and one visiting period at the Dipartimento di Matematica e Informatica “Ulisse Dini”, Università degli Studi di Firenze, under the supervision of Prof. Luigi Barletti. The results of this collaboration are in preprint form [8] and they are partially illustrated in this thesis. A second topic concerns the optimal control theory of charge transport in graphene. The preliminary results presented in this thesis have been developed during a visiting period at the Institut für Mathematik, Julius-Maximilians-Universität Würzburg, under the supervision of Prof. A. Borzi. During this period, we began our analysis about the Boltzmann equation with a study of an optimization problem involving the Keilson-Storer master equation, solved by a Monte Carlo approach. The collaboration has led to the preprint [11] not mentioned in this thesis in detail because it does not concern the charge transport in graphene.

Finally, we would like to mention two ongoing works. The first one regards the electron-electron interaction in the semiclassical Boltzmann model [28], the second one proposes a non homogeneous numerical solution of the semiclassical Boltzmann equation with the DG method to simulate the current in a GFET [79]. Both the works are still in a preprint version and they have been presented at the 26th International Congress on Transport Theory (ICTT-26), held in Paris in September 2019.

The plan of the thesis is as follows. In Chapter 1 we describe some basic aspects about charge transport in graphene and introduce in detail the physical models we will adopt. In Chapter 2 we describe all the numerical methods chosen to get our simulations. Different approaches have been adopted depending on the cases to treat. Chapter 3 is devoted to the bipolar charge transport in graphene, where both the contributions to the current due to electrons and holes and the inter-band transitions of carriers are taken into account [63, 27]. In Chapter 4 we focus first on the improvements of mobility models in suspended monolayer graphene [81] and then in the case

of graphene placed on a substrate [79]. Since a crucial parameter is the distance between the graphene layer and the impurities of the substrate, some simulations based on stochastic models have been performed by means of DSMC [24]. Finally a Graphene Field Effect Transistor (GFET) is simulated by solving the drift-diffusion equations adopting a mobility model based on experimental data [82] and the ones mentioned above based on the semiclassical Boltzmann equation [79]. Chapter 5 regards the classical-quantum drift diffusion model of charge transport in graphene. In Chapter 6 we present the optimal control theory of charge transport in graphene. Chapter 7 consists of two short parts regarding subjects still under investigation, the first one regarding the electron-electron interaction in the semiclassical Boltzmann model, the second one proposing numerical solution of the semiclassical Boltzmann equation for a GFET by means of a DG approach.

Chapter 1

Charge transport in graphene

Low dimensional materials are widely investigated to reduce the size of new electron devices. One of the most prominent is graphene because of its singular electronic properties, such as the very high conductivity. The main idea is to adapt mathematical models already developed for Si and GaAs based electron devices to graphene ones. One of the most accurate is the semiclassical Boltzmann equations where quantum aspects are also taken into account. Since numerical solutions of the Boltzmann equations require a high computational effort, macroscopic models have been formulated such as drift-diffusion, energy-transport or hydrodynamical. They constitute a more useful tool to design, improve and optimize new graphene based electron devices.

In this chapter we present the physical properties of graphene and the mathematical models adopted to simulate the charge transport. For a more exhaustive discussion regarding the charge transport in low dimensional structures see [17]. In Section 1.1 we introduce some basic notions about solid state physics and in Section 1.2 we present the structure of graphene. As mathematical model we introduce the semiclassical Boltzmann equation, treated in Section 1.3, and the drift-diffusion model, outlined in Section 1.4.

1.1 Solid state physics basic concepts

Solid state physics is the branch of physics that studies physical properties of solid matter resulting from the distribution of electrons in metals, semiconductors, and insulators. Solid materials are formed from high concentrated atoms interacting each other. These interactions produce the mechanical, thermal, electrical, magnetic and optical properties of solids. Crystals constitute a particular class of solids material formed by identical building blocks of atoms or group of atoms. Such periodic structure allows a more detailed mathematical description. However, for our purpose we concentrate on the conductivity property.

In this section we focus on the basic definitions in solid state physics and on electron transport in solids from the microscopic description to the statistical one. For further

informations the reader is referred to some classical textbooks about solid state physics [4, 52, 110, 44].

1.1.1 Crystal lattices

Solid state materials satisfy two more major properties: distances between atoms are small (about 10^{-10}m) and equilibrium positions of atoms are fixed. Depending on the shape of equilibrium configurations, the solid has or has not a regular structure. In a crystal all the points related by specific translation vectors $\mathbf{r}_n$ are equivalent. More in details, if

$$\mathbf{r}' = \mathbf{r} + \mathbf{r}_n,$$

then $\mathbf{r}' \equiv \mathbf{r}$ and all physical quantities assume the same value both in $\mathbf{r}$ and in $\mathbf{r}'$.

We define crystal lattice a countable subset R of $\mathbb{R}^d$, with $d = 1, 2, 3$, spanned by d independent vectors $\mathbf{a}_1, \dots, \mathbf{a}_d$, that is

$$R = \left\{ \mathbf{a} \in \mathbb{R}^d \mid \mathbf{a} = n_1 \mathbf{a}_1 + \dots + n_d \mathbf{a}_d, \quad n_1, \dots, n_d \in \mathbb{Z} \right\}. \quad (1.1)$$

Moreover the set $\{\mathbf{a}_1, \dots, \mathbf{a}_d\}$ is called basis of R , and the vectors $\mathbf{a}_i$ per $i = 1, \dots, d$ are called primitive vectors generating R .

We define primitive cell of R a subset $\mathcal{D}_R$ of $\mathbb{R}^d$ containing only one element of R (usually the origin) such that its translations covers $\mathbb{R}^d$.

We define unit cell the primitive cell defined only by minimal length vectors, that is explicitly

$$\mathcal{D} = \left\{ \mathbf{x} = \alpha_1 \mathbf{a}_1 + \dots + \alpha_d \mathbf{a}_d, \text{ with } \alpha_1, \dots, \alpha_d \in [0, 1[\right\}.$$

We define Wigner-Seitz primitive cell the region $\mathcal{D}_{WS}$ around the origin whose points are nearer to the origin with respect to every other lattice point, that is

$$\mathcal{D}_{WS} = \left\{ \mathbf{x} \in \mathbb{R}^d \mid |\mathbf{x}| \leq |\mathbf{x} + \mathbf{a}|, \forall \mathbf{a} \in R \right\}.$$

To better clarify the previous definition we consider the Figure 1.1.

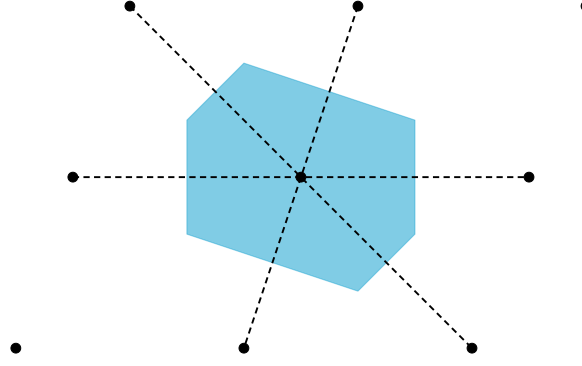


FIGURE 1.1: Representation of the Wigner-Seitz primitive cell for a two-dimensional crystal lattice (see [4]).

Crystal lattices are classified in relation of their translation properties. Let us consider a translation $T_{\mathbf{a}} : \mathbb{R}^d \rightarrow \mathbb{R}^d$ defined by

$$T_{\mathbf{a}}(\mathbf{x}) = \mathbf{x} + \mathbf{a}.$$

Therefore we have that $T_{\mathbf{a}}(R) = R$, $\forall \mathbf{a} \in R$ and, on the other hand, a lattice is translation invariant if and only if it is translated with respect to an own element. It is possible to prove that there exists a finite number of types of translation lattices, called Bravais lattices. In one dimensional case there exists only one Bravais lattice, in two dimensions there are 5 and in three dimensions there exists 14 (see [4]).

Given a translation lattice R having basis $\{\mathbf{a}_1, \dots, \mathbf{a}_d\}$, we define the reciprocal lattice G having basis $\{\mathbf{b}_1, \dots, \mathbf{b}_d\}$ where these vectors defined by

$$\mathbf{b}_i \cdot \mathbf{a}_j = 2\pi\delta_{ij}, \quad (1.2)$$

with δ_{ij} the Kronecker symbol.

We remark that $\mathbf{b}_1, \dots, \mathbf{b}_d$ are d vectors each of one is orthogonal to all the element of R basis except one. Therefore $\{\mathbf{b}_1, \dots, \mathbf{b}_d\}$ is a basis of $\mathbb{R}^d$ and the set

$$G = \left\{ \mathbf{x} \in \mathbb{R}^d \mid \mathbf{x} = m_1\mathbf{b}_1 + m_d\mathbf{b}_d, \text{ with } m_1, \dots, m_d \in \mathbb{Z} \right\}$$

define another crystal lattice. We remark that if R is a Bravais lattice then also G it is.

We define the first Brillouin zone the Wigner-Seitz primitive cell of the reciprocal lattice, that is

$$\mathcal{B} = \left\{ \mathbf{k} \in \mathbb{R}^3 \mid |\mathbf{k}| \leq |\mathbf{k} + \mathbf{b}| \quad \forall \mathbf{b} \in G \right\}. \quad (1.3)$$

The center of the first Brillouin zone is called Γ point.

1.1.2 Electrons and phonons

A free atom consists of a nucleus surrounded by closed shells of electrons and one or more valence electrons around them. The mass of the atom is assumed to be concentrated at its nucleus and the closed shells form a halo of charge around the core. The valence electrons move by effect of the electric field generated by the nucleus particles. If we bring the atoms together to make a crystalline lattice, the valence electrons move under the electric field generated by all the ions. The valence electrons are not bounded to their original atom but they can move in all the lattice and they are responsible for the electrical conduction.

Nuclei of atoms constituting the crystal lattice are not fixed, but they oscillate around their equilibrium positions. These oscillations propagate into the lattice as waves. The oscillation modes are called phonons, whose frequency is indicated by ω . They can assume only discrete values of energy,

$$\varepsilon_n = (n + 1/2)\hbar\omega, \quad n = 0, 1, 2, \dots, \quad (1.4)$$

where $\hbar$ is the reduced Planck constant. If an electron interacts with a phonon a scattering occurs and its state changes. If it happens a transition from the state ε_n to ε_{n-1} then an absorption occurs, if there is a transition from ε_n to ε_{n+1} then there is an emission. Vibration modes in crystals are classified in two main classes: optical waves and acoustic waves.

In the Debye approximation, acoustic waves have a linear dispersion relation, that is

$$\hbar\omega_{ac}(|\mathbf{k}|) \approx c_s \hbar|\mathbf{k}|, \quad (1.5)$$

where c_s is the sound speed in the crystal. In the Einstein approximation, Optical waves have a constant dispersion relation, that is

$$\hbar\omega_{op}(|\mathbf{k}|) \approx \hbar\omega_{op}. \quad (1.6)$$

1.1.3 Electron transport in solids

Let us suppose to have a system composed by N electrons. To determine the eigenstates of the system, we need to find a function Ψ of the coordinates $\mathbf{x}_i$, $i = 1, 2, \dots, N$ such that

$$\left\{ \sum_i \frac{1}{2m} \mathbf{p}_i^2 + \sum_i \mathcal{U}(\mathbf{x}_i) + \sum_{i,j} \frac{e^2}{|\mathbf{x}_i - \mathbf{x}_j|} \right\} \Psi(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N) = \mathcal{E} \Psi(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N), \quad (1.7)$$

being m the electron mass, $\mathbf{p}_i$ the momentum of each electron and e the elementary charge. The momentum is related to the wave vector by $\mathbf{p}_i = \hbar \mathbf{k}_i$. In the left hand side, the first term represents the kinetic energy, the second one the potential energy due to the ions and the third one the interaction energy. In quantum mechanics the kinetic energy term can be written as an operator by means of

$$\frac{1}{2m} |\mathbf{p}_i|^2 \longrightarrow -\frac{\hbar^2}{2m} \nabla_i^2. \quad (1.8)$$

The full description of an electronic state requires also a knowledge of the spin of the electron. This properties classifies electrons in two classes: those that have spin $1/2$ and those having spin $-1/2$.

The equation (1.7) is extremely complicated to solve, in particular for the presence of the interaction term. A first rough approximation consists to take into account only kinetic energy and neglect the other terms. This is called free electron model. In this way the system is described as a gas of free electrons. This model can be suitable for alkali metals in which there is only one valence electron outside the closed shell that behaves as free.

To have a deeper knowledge of the structure of solids it is necessary to consider also the potential energy in (1.7). By neglecting the interaction term we remark that the wave function of the system can be separate into factors, each corresponding to the coordinates of a single electron. This fact leads to the single Schrödinger equation

$$\left\{ -\frac{\hbar^2}{2m} \nabla^2 + \mathcal{U}(\mathbf{x}) \right\} \psi(\mathbf{x}) = \mathcal{E} \psi(\mathbf{x}). \quad (1.9)$$

In general no exact solutions are known but one must resort to numerical procedures. Since in a crystal ions are arranged in a periodic structure we can assume that the potential $\mathcal{U}(\mathbf{x})$ is periodic, that is

$$\mathcal{U}(\mathbf{x} + \mathbf{T}) = \mathcal{U}(\mathbf{x}), \quad (1.10)$$

for all translation vectors $\mathbf{T}$. Under the previous hypothesis, Bloch's theorem states that the eigenstates of the Hamiltonian appearing in (1.8), that we indicate by $\mathcal{H}^0$ from now on, can be chosen to have the form of a plane wave times a function with the periodicity of the lattice, that is

$$\psi_{n,\mathbf{k}}(\mathbf{x}) = e^{i\mathbf{k} \cdot \mathbf{x}} u_{n,\mathbf{k}}(\mathbf{x}),$$

where

$$u_{n,\mathbf{k}}(\mathbf{x} + \mathbf{T}) = u_{n,\mathbf{k}}(\mathbf{x}),$$

for all translation vectors $\mathbf{T}$. For a proof of Bloch's theorem see [4]. The quantum number $\mathbf{k}$ characterizes the translation symmetry of the potential. Due to the periodicity, it can be thought as confined in the first Brillouin zone. If multiplied by $\hbar$ it is called crystal momentum. The index n appears because given $\mathbf{k}$ there are many solution of the equation (1.8). This index varies discretely. In terms of eigenvalues we remark that the levels of an electron in a periodic potential are described by a family of continuous functions $\mathcal{E}_n(\mathbf{k})$, each one called band and all of them together constitute the electronic band structure of the solid. Moreover an electron of wavevector $\mathbf{k}$ belonging in an energy level labeled by n has a mean velocity given by

$$\mathbf{v}_n(\mathbf{k}) = \frac{1}{\hbar} \nabla_{\mathbf{k}} \mathcal{E}_n(\mathbf{k}).$$

We can characterize insulators by the energy gap, that is the difference between the top of the highest filled bands and the bottom of the lowest empty bands. Let us sort the bands by increasing energies. At zero absolute temperature a solid with an energy gap is nonconducting. When the temperature is not zero there is a nonvanishing probability that some electrons will be thermally excited across the energy gap into the lowest unoccupied bands, which are called, in this context, the conduction bands, leaving behind unoccupied levels in the highest occupied bands, called valence bands. If the gap is much higher than $k_B T$, where k_B is the Boltzmann constant and T is the room temperature, the material is an insulator. If the energy gap is comparable with $k_B T$, the material is an intrinsic semiconductor. If the last occupied band is only partially occupied, the material is a metallic conductor. The energy of the topmost filled orbital at absolute zero is called Fermi energy and indicated by ε_F . The points in $\mathbf{k}$ -space where carriers have minimum energy are called valleys.

Now let we suppose to have a field of force with Hamiltonian $\mathcal{H}'$ acting on electrons. The motion governed by the combined Hamiltonian $\mathcal{H}^0$ and $\mathcal{H}'$ satisfies the time-dependent Schrödinger equation

$$(\mathcal{H}' + \mathcal{H}^0)\psi(\mathbf{x}, t) = i\hbar \frac{\partial}{\partial t} \psi(\mathbf{x}, t) \quad (1.11)$$

or equivalently (see [110])

$$\{\mathcal{H}' + \mathcal{E}(-i\nabla)\} \psi(\mathbf{x}, t) = i\hbar \frac{\partial}{\partial t} \psi(\mathbf{x}, t). \quad (1.12)$$

We remark that a wave-packet solution of (1.12) has exactly the same trajectory as

a particle obeying the equations derived from the appropriate classical Hamiltonian. The latter is obtained by replacing the operator $-i\hbar\nabla$ by the classical momentum $\mathbf{p}$,

$$\mathcal{H}(\mathbf{x}, \mathbf{p}) = \mathcal{H}'(\mathbf{x}, \mathbf{p}) + \mathcal{E}\left(\frac{\mathbf{p}}{\hbar}\right). \quad (1.13)$$

Let us assume that the external force is due to a space dependent electrostatic potential $V(\mathbf{x})$, then we have

$$\mathcal{H}'(\mathbf{x}, \mathbf{p}) = -eV(\mathbf{x}),$$

being e the elementary charge in absolute value. Moreover, if we assume that $\mathbf{p}$ is the crystal momentum we get the so called semiclassical approximation, leading to the following equations of motion

$$\dot{\mathbf{x}} = \mathbf{v}_n(\mathbf{k}), \quad \dot{\mathbf{k}} = \frac{e}{\hbar} \nabla_{\mathbf{x}} V(\mathbf{x}). \quad (1.14)$$

The above mentioned assumption is not properly physically justified. The interested reader is referred to [49] for example. Let us consider a gas of semiclassical electrons each one satisfying (1.14). From the Liouville evolution equation for the phase space distribution function, by adapting the well known procedure for rarefied gas, see [65], we get the semiclassical Vlasov equation

$$\frac{\partial f}{\partial t} + \mathbf{v}(\mathbf{k}) \cdot \nabla_{\mathbf{x}} f - \frac{e}{\hbar} \mathbf{E}(t, \mathbf{x}) \cdot \nabla_{\mathbf{k}} f = 0, \quad (1.15)$$

being $\mathbf{E}(t, \mathbf{x}) = -\nabla_{\mathbf{x}} V(t, \mathbf{x})$ and where distribution function $f(t, \mathbf{x}, \mathbf{k})$ is defined in such a way that $f(t, \mathbf{x}, \mathbf{k}) d\mathbf{x} d\mathbf{k}$ indicates the number of particles with positions in the volume $d\mathbf{x}$ around $\mathbf{x}$ and wavevector in $d\mathbf{k}$ around $\mathbf{k}$, at time t .

To incorporate in the equation the quantum effects of the semiconductor crystal lattice, such as electron-phonon, electron-substrate and electron-electron scatterings, we include on the right hand side a collision term $Q(f)$, whose expression will be given in details in the next, leading to the semiclassical Boltzmann equation

$$\frac{\partial f}{\partial t} + \mathbf{v}(\mathbf{k}) \cdot \nabla_{\mathbf{x}} f - \frac{e}{\hbar} \mathbf{E}(t, \mathbf{x}) \cdot \nabla_{\mathbf{k}} f = Q(f). \quad (1.16)$$

1.1.4 Equilibrium distributions

To describe a gas of identical particles in quantum terms, we must consider the statistical ensemble of systems formed by the entire gas. For a gas of bosons, there is the possibility to find any number of particles in the same quantum state. The average occupation number in a single-particle state with energy ε_i is given by the Bose-Einstein

distribution

$$\bar{n}_i = \frac{1}{\exp\left(\frac{\varepsilon_i - \mu}{k_B T}\right) - 1}, \quad (1.17)$$

where μ is the chemical potential. If the particles are fermions, by the Pauli exclusion principle, we know that two particles cannot occupy the same state. The average occupation number in a single-particle state with energy ε_i is given by the Fermi–Dirac distribution

$$\bar{n}_i = \frac{1}{\exp\left(\frac{\varepsilon_i - \mu}{k_B T}\right) + 1}. \quad (1.18)$$

In this case the chemical potential μ is also called Fermi level [44], indicated by ε_F .

1.2 Graphene structure

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 [7, 19, 56, 73] and optoelectronic devices [109]. Graphene is a material having many interesting physical properties (see [19], [99], [38]). Electrons in graphene behave as relativistic massless particles (Dirac fermions). This fact furnishes many peculiar properties such as the quantum anomalous Hall effect and the absence of localization. Further graphene properties are the high electron mobility at room temperature ($250\,000\text{ cm}^2/\text{Vs}$), the elevated thermal conductivity ($5000\text{ Wm}^{-1}\text{K}^{-1}$) and the unique mechanical properties with a Young modulus of 1 TPa.

In order to have a complete setting it is fundamental to describe the crystal structure and the energy band of graphene.

Graphene is a single layer of carbon (C) atoms arranged in a two dimensional honeycomb lattice (see [38]). Graphene is the basic element for other materials deriving from graphite: it can be wrapped in fullerene (0D), rolled in carbon nanotube (1D) or piled in graphite (3D). Moreover another possible configuration is the graphene nanoribbon (GNR) consisting of a strip having a sufficiently small width such that electrons are confined in one direction.

Graphene is composed by carbon atoms. Carbon is a chemical element with 6 protons and 6 electrons, 2 core and 4 valence electrons. The electron configuration of carbon is given by 1s and 2s orbitals completely filled and two 2p orbitals containing one electron. In compact form the fundamental state of carbon is $1s^2 2s^2 2p^1$. In graphene each atom has a covalent bond with other two carbon atoms. Thus each atom has three hybrid orbitals sp^2 staying on the same plane e forming angles of 120° . The fourth

electron stays in a $2p_z$ orbital, which axis is perpendicular with respect to the plane of the three others. It generates the electronic bands (see [19]).

1.2.1 The honeycomb lattice

Graphene is described by a two dimensional honeycomb lattice in whose vertices are arranged the carbon atoms. The crystal structure and the electronic energy band have been first studied by [105] and then summarized by [19]. The honeycomb net is classified as a triangular Bravais lattice with a two-point basis [4]. In this way it can be considered as composed by two interpenetrating nonequivalent sublattices, usually indicated by A and B . The primitive vectors are

$$\mathbf{a}_1 = \frac{a}{2}(3, \sqrt{3}), \quad \mathbf{a}_2 = \frac{a}{2}(3, -\sqrt{3}), \quad (1.19)$$

where $a \approx 1.42\text{\AA}$ is the nearest neighbor distance. Since we have a two-point basis this is not the lattice constant, that is $a\sqrt{3} \approx 2.46\text{\AA}$. Regarding the sublattice A , the nearest neighbors are located through the vectors

$$\boldsymbol{\delta}_1 = \frac{a}{2}(1, \sqrt{3}), \quad \boldsymbol{\delta}_2 = \frac{a}{2}(1, -\sqrt{3}), \quad \boldsymbol{\delta}_3 = -a(1, 0) \quad (1.20)$$

and, similarly, for sublattice B they are

$$\boldsymbol{\gamma}_1 = -\frac{a}{2}(1, \sqrt{3}), \quad \boldsymbol{\gamma}_2 = \frac{a}{2}(-1, \sqrt{3}), \quad \boldsymbol{\gamma}_3 = a(1, 0). \quad (1.21)$$

In the Figure 1.2 the above mentioned properties are depicted, where the sublattices A and B are colored in yellow and red respectively and the unit cell is highlighted in blue. The primitive reciprocal vectors of are

$$\mathbf{b}_1 = \frac{2\pi}{3a}(1, \sqrt{3}), \quad \mathbf{b}_2 = \frac{2\pi}{3a}(1, -\sqrt{3}). \quad (1.22)$$

They define an hexagonal Brillouin zone, represented in Figure 1.3. Let us consider a reference frame whose origin is the Γ point, that is the center of the Brillouin zone. The vertices of the latter, indicated by $\mathbf{K}$ e $\mathbf{K}'$ and called Dirac points, are located in

$$\mathbf{K} = \left(\frac{2\pi}{3a}, \frac{2\pi}{3\sqrt{3}a} \right), \quad \mathbf{K}' = \left(\frac{2\pi}{3a}, -\frac{2\pi}{3\sqrt{3}a} \right). \quad (1.23)$$

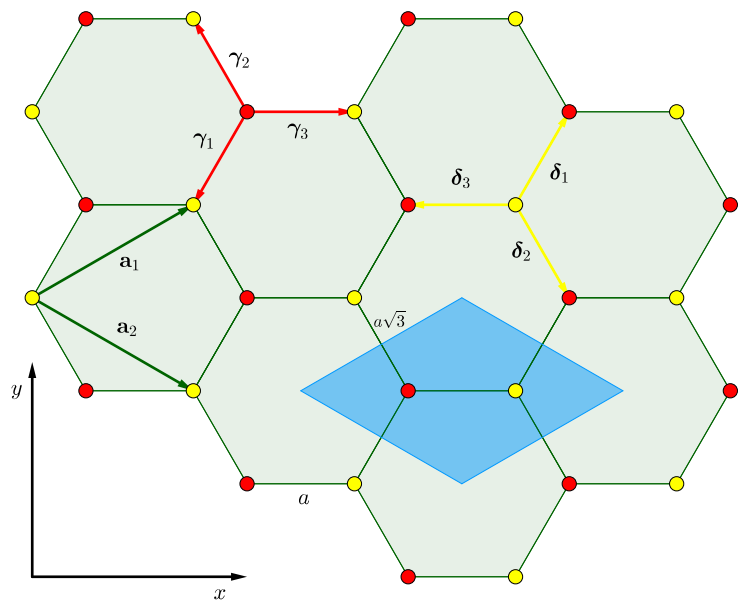


FIGURE 1.2: Structure of graphene honeycomb lattice.

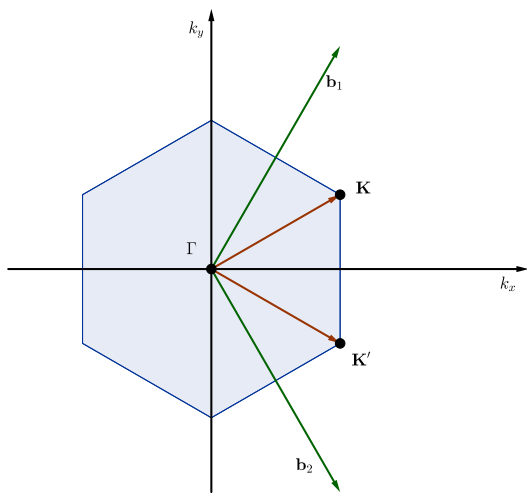


FIGURE 1.3: The Brillouin zone.

1.2.2 The electronic band structure

The energy bands are derived from the tight-binding Hamiltonian for electrons in graphene, considering that electrons can hop to both nearest- and next-nearest-neighbor atoms. They have the form (see [19])

$$E_{\pm}(\mathbf{k}) = \pm\gamma_1\sqrt{3 + f(\mathbf{k})} - \gamma_2 f(\mathbf{k}), \quad (1.24)$$

with

$$f(\mathbf{k}) = 2 \cos\left(\sqrt{3}k_y a\right) + 4 \cos\left(\frac{\sqrt{3}}{2}k_y a\right) \cos\left(\frac{3}{2}k_x a\right), \quad (1.25)$$

where $\gamma_1 \approx 2.8 \text{ eV}$ is the nearest-neighbor hopping energy and $\gamma_2 \approx 0.1 \text{ eV}$ is the next nearest-neighbor hopping energy. We remark that the coordinates of $\mathbf{k}$ are expressed with respect to the Γ point. In the Equation (1.24) the plus sign corresponds to the conduction band π^* and the minus sign refers to the valence band π . If we neglect the next nearest-neighbor hopping energy, that is we assume $\gamma_2 = 0$, the two bands appear to be symmetrical. In this case by simple calculation we can assert that the two energy bands touches at the Dirac points. It means that there is no energy gap in graphene. Moreover, by expanding the full band structure (1.24) close to $\mathbf{K}$ (or $\mathbf{K}'$) the dispersion relation reduces to

$$E_{\pm}(\mathbf{k}) \approx \pm\hbar v_F |\mathbf{k}| + \mathcal{O}(|\mathbf{k}|^2), \quad (1.26)$$

where v_F is the Fermi velocity, given by

$$v_F = \frac{3\gamma_1 a}{2\hbar}, \quad (1.27)$$

with a value of $v_F \approx 10^6 \text{ m/s}$. Therefore we remark that the dispersion relation shape is conic near the Dirac points. A plot is shown in Figure 1.4.

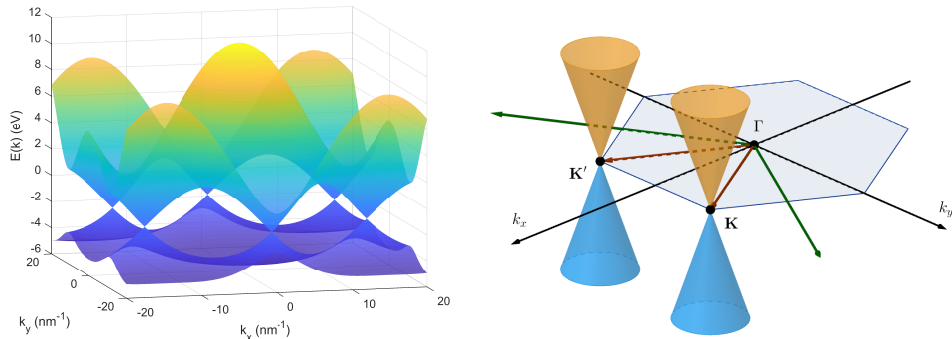


FIGURE 1.4: Electronic dispersion in the honeycomb lattice. The full expression is reproduced on the left, the zoom in close the Dirac points is shown on the right.

1.3 The semiclassical Boltzmann equation

The first kinetic equation for particle distribution function in dilute classical gases has been devised by [13]. To describe the electron transport in solids a variant, based on the assumption of particles obeying to the Fermi-Dirac distribution, has been proposed the first time by [102]. Thereafter, the semiclassical Boltzmann model has been refined by taking into account many effects.

In a semiclassical kinetic setting, the charge transport in graphene is described, in general, by four Boltzmann equations, one for electrons in the valence (π) band and one for electrons in the conduction (π^*) band, that in turn can belong to the K or K' valley. By assuming the K and K' valleys as equivalent, then we can consider only the two equations

$$\frac{\partial f_s}{\partial t} + \mathbf{v}_s \cdot \nabla_{\mathbf{x}} f_s - \frac{e}{\hbar} \mathbf{E} \cdot \nabla_{\mathbf{k}} f_s = Q(f_s, f_{-s}) \quad (s = \pm 1), \quad (1.28)$$

where $f_s = f_s(\mathbf{t}, \mathbf{x}, \mathbf{k})$ represents the distribution function of charge carriers in the conduction band (CB), for $s = 1$, or in the valence band (VB), for $s = -1$, at position $\mathbf{x} \in U \subset \mathbb{R}^2$, time t and wave-vector $\mathbf{k} \in \mathbb{R}^2$. We denote by $\nabla_{\mathbf{x}}$ and $\nabla_{\mathbf{k}}$ the gradients with respect to the position and wave vector, respectively. In the sequel, for simplifying the notation, we write also f_+ and f_- to indicate the distributions of electrons in the conduction and valence bands.

The group velocity $\mathbf{v}_s$ is related to the energy band ε_s by

$$\mathbf{v}_s = \frac{1}{\hbar} \nabla_{\mathbf{k}} \varepsilon_s.$$

As said, with a very good approximation, in [19], a linear dispersion relation holds for the energy bands ε_s around the Dirac points; so that, choosing the origin of the reference frame in the $\mathbf{k}$ -space coinciding with a Dirac point, we have $\varepsilon_s = s \hbar v_F |\mathbf{k}|$, where v_F is the (constant) Fermi velocity and $\hbar$ the Planck constant divided by 2π . The elementary (positive) charge is denoted by e . The electric field $\mathbf{E}(\mathbf{t}, \mathbf{x})$ is related to the electrostatic potential $\phi(\mathbf{t}, \mathbf{x})$ through

$$\mathbf{E} = -\nabla_{\mathbf{x}} \phi, \quad (1.29)$$

where $\phi(\mathbf{t}, \mathbf{x})$ might be external or recovered by coupling (1.28) with a Poisson equation. The right hand side of Eq. (1.28) is the collision term due to several kinds of scatterings. It can be thought as

$$Q(f_s, f_{-s}) = Q^{(el-ph)}(f_s, f_{-s}) + Q^{(el-sub)}(f_s, f_{-s}) + Q^{(el-el)}(f_s, f_{-s})$$

where $Q^{(el-ph)}$ represents the interaction of electrons with acoustic, optical and K phonons; $Q^{(el-sub)}$ describes the scatterings of electrons with optical phonons and impurities of a substrate where the graphene layer is placed on; $Q^{(el-el)}$ represents the electron-electron interaction.

In the valence band, instead of electrons, it is possible to consider holes. If we indicate with $\mathbf{k}_e$ the state of a missing electron in the VB and with $\mathbf{k}_h$ and $\varepsilon_h(\mathbf{k}_h)$ the state and the energy of the corresponding hole, they are related by the conditions [52, 44]

$$\mathbf{k}_h = -\mathbf{k}_e, \quad \varepsilon_h(\mathbf{k}_h) = -\varepsilon_-(\mathbf{k}_e).$$

Removing the labels to avoid unnecessarily complicated notation, the dispersion relation for the energy of holes writes

$$\varepsilon_h(\mathbf{k}) = \hbar v_F |\mathbf{k}|.$$

The distribution function of holes in the VB is defined by

$$f_h(\mathbf{t}, \mathbf{x}, \mathbf{k}) = 1 - f_-(\mathbf{t}, \mathbf{x}, -\mathbf{k}).$$

We close the description of the semiclassical Boltzmann equation by presenting a special case. Let us consider the ideal physical situation, depicted in Fig. 1.5, of a graphene sheet of length L and infinitely large with two parallel metallic contacts placed at the extremities of its length. If a fixed bias voltage V_b is applied then a linear electrostatic

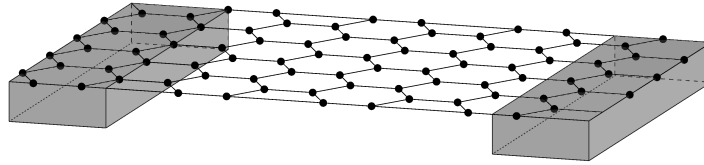


FIGURE 1.5: Schematic representation of a suspended monolayer graphene with metallic contacts.

potential is generated between the two contacts and therefore the corresponding electric field reads

$$\mathbf{E} = -\frac{V_b}{L} \mathbf{u},$$

being $\mathbf{u}$ the unit vector directed perpendicularly to the contacts. Since the electric field is constant, the dependence on $\mathbf{x}$ disappears in the Boltzmann equation, which becomes

$$\frac{\partial f_s}{\partial \mathbf{t}} - \frac{e}{\hbar} \mathbf{E} \cdot \nabla_{\mathbf{k}} f_s = Q(f_s, f_{-s}) \quad (s = \pm 1), \quad (1.30)$$

where now $f_s = f_s(t, \mathbf{k})$ and we will refer to this situation as spatially homogeneous case.

About analytic results on the semiclassical Boltzmann equation space homogeneous solutions to the Cauchy problem have been obtained in [61], a result on global existence and uniqueness of smooth solutions in two dimensions and locally in three dimensions can be found in [78]. In [84] global existence and uniqueness of smooth solutions in any dimension for a system when the wave vector belongs to the bounded Brillouin zone has been shown. In [57] even the electric field is controlled and in [3] the collision term and the dependence of the energy band diagram is also taken into account.

1.3.1 Electron-phonon interactions

Acoustic phonon scattering (ac) is intra-valley and intra-band. Optical phonon scattering is intra-valley and can be longitudinal optical (LO) and transversal optical (TO); it can be intra-band, that is leaves the electron in the same band, or inter-band pushing the electron from an initial band to the other one. Scattering with optical phonon of type K pushes electrons from a valley to a neighbor one (inter-valley scattering). Hence, the general form of Q^{el-ph} can be written as

$$Q^{(el-ph)}(f_s, f_{-s})(t, \mathbf{x}, \mathbf{k}) = \sum_{s'} \left[\int_{\mathbb{R}^2} S_{s',s}^{(el-ph)}(\mathbf{k}', \mathbf{k}) f_{s'}(t, \mathbf{x}, \mathbf{k}') (1 - f_s(t, \mathbf{x}, \mathbf{k})) d\mathbf{k}' \right. \\ \left. - \int_{\mathbb{R}^2} S_{s,s'}^{(el-ph)}(\mathbf{k}, \mathbf{k}') f_s(t, \mathbf{x}, \mathbf{k}) (1 - f_{s'}(t, \mathbf{x}, \mathbf{k}')) d\mathbf{k}' \right]$$

where the total transition rate is given by the sum of the contributions of the several types of scatterings

$$S_{s',s}^{(el-ph)}(\mathbf{k}', \mathbf{k}) = \sum_{\nu} \left| G_{s',s}^{(\nu)}(\mathbf{k}', \mathbf{k}) \right|^2 \left[\left(n_{\mathbf{q}}^{(\nu)} + 1 \right) \delta \left(\varepsilon_s(\mathbf{k}) - \varepsilon_{s'}(\mathbf{k}') + \hbar \omega_{\mathbf{q}}^{(\nu)} \right) \right. \\ \left. + n_{\mathbf{q}}^{(\nu)} \delta \left(\varepsilon_s(\mathbf{k}) - \varepsilon_{s'}(\mathbf{k}') - \hbar \omega_{\mathbf{q}}^{(\nu)} \right) \right]. \quad (1.31)$$

The index ν labels the ν th phonon mode, $\left| G_{s',s}^{(\nu)}(\mathbf{k}', \mathbf{k}) \right|$ is the matrix element, which describes the scattering mechanism, due to phonons of type ν , between electrons belonging to the band s' and electrons belonging to the band s . The symbol δ denotes the Dirac distribution, $\omega_{\mathbf{q}}^{(\nu)}$ is the ν th phonon frequency, $n_{\mathbf{q}}^{(\nu)}$ is the Bose-Einstein distribution for the phonon of type ν

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

k_B is the Boltzmann constant and T is the graphene lattice temperature. We assume that phonons are at thermal equilibrium, then the lattice temperature will be kept constant. When, for a phonon ν_* , $\hbar \omega_{\mathbf{q}}^{(\nu_*)} \ll k_B T$, then the scattering with the phonon ν_* can be assumed elastic. In this case, we eliminate in Eq. (1.31) the term $\hbar \omega_{\mathbf{q}}^{(\nu_*)}$ inside the delta distribution and we use the approximation $n_{\mathbf{q}}^{(\nu_*)} + 1 \approx n_{\mathbf{q}}^{(\nu_*)}$.

Now we write explicitly the transition rates used in our simulations.

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

$$2 n_{\mathbf{q}}^{(ac)} \left| G^{(ac)}(\mathbf{k}', \mathbf{k}) \right|^2 = \frac{1}{(2\pi)^2} \frac{\pi D_{ac}^2 k_B T}{2\hbar \sigma_m v_p^2} (1 + \cos \vartheta_{\mathbf{k}, \mathbf{k}'}), \quad (1.32)$$

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

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

$$\left| G^{(LO)}(\mathbf{k}', \mathbf{k}) \right|^2 + \left| G^{(TO)}(\mathbf{k}', \mathbf{k}) \right|^2 = \frac{2}{(2\pi)^2} \frac{\pi D_O^2}{\sigma_m \omega_O} \quad (1.33)$$

$$\left| G^{(K)}(\mathbf{k}', \mathbf{k}) \right|^2 = \frac{1}{(2\pi)^2} \frac{2\pi D_K^2}{\sigma_m \omega_K} (1 - \cos \vartheta_{\mathbf{k}, \mathbf{k}'}), \quad (1.34)$$

where D_O is the optical phonon coupling constant, ω_O the optical phonon frequency, D_K is the K-phonon coupling constant and ω_K the K-phonon frequency. Physical parameters for the collision terms are summarized in Table 1.1.

v_F	10^8 cm/s	v_p	2×10^6 cm/s
σ_m	7.6×10^{-8} g/cm ²	D_{ac}	6.8 eV
$\hbar \omega_O$	164.6 meV	D_O	10^9 eV/cm
$\hbar \omega_K$	124 meV	D_K	3.5×10^8 eV/cm

TABLE 1.1: Physical parameters for the (el-ph) collision term.

1.3.2 Electron-substrate interactions

Remote optical phonon scattering is intra-valley and can be longitudinal optical (LO-sub) and transversal optical (TO-sub); it can be also intra-band or inter-band. Remote impurity scattering (imp) is intra-valley and intra-band.

Regarding the electron substrate scatterings, the collision term $Q^{(el-sub)}$ has the same form of $Q^{(el-ph)}$ and the total transition rate (1.31) is given by

$$S_{s',s}^{(el-sub)}(\mathbf{k}', \mathbf{k}) = S_{s',s}^{(O-sub)}(\mathbf{k}', \mathbf{k}) + S_{s',s}^{(imp)}(\mathbf{k}', \mathbf{k}) \quad (1.35)$$

where

$$S_{s',s}^{(O-sub)}(\mathbf{k}', \mathbf{k}) = \left| G^{(O-sub)}(\mathbf{k}', \mathbf{k}) \right|^2 \left[\left(n_{\mathbf{q}}^{(O-sub)} + 1 \right) \delta \left(\varepsilon_s(\mathbf{k}) - \varepsilon_{s'}(\mathbf{k}') + \hbar \omega_{\mathbf{q}}^{(O-sub)} \right) + n_{\mathbf{q}}^{(O-sub)} \delta \left(\varepsilon_s(\mathbf{k}) - \varepsilon_{s'}(\mathbf{k}') - \hbar \omega_{\mathbf{q}}^{(O-sub)} \right) \right],$$

being

$$\left| G^{(O-sub)}(\mathbf{k}', \mathbf{k}) \right|^2 = \left| G^{(LO-sub)}(\mathbf{k}', \mathbf{k}) \right|^2 + \left| G^{(TO-sub)}(\mathbf{k}', \mathbf{k}) \right|^2 = \frac{2}{(2\pi)^2} \frac{\pi D_{O-sub}^2}{\sigma_m \omega_{O-sub}}.$$

Moreover, concerning $S_{s',s}^{(imp)}$, we assume that the remote impurities stay in a plane at distance d from the graphene sheet. The definition of the scattering rate for electron-impurity scattering is highly complex; so many approximate models are proposed. Following [43], we adopt the expression

$$S_{s',s}^{(imp)}(\mathbf{k}, \mathbf{k}') = \frac{2\pi}{\hbar} \frac{n_i}{(2\pi)^2} \left| \frac{V_i(|\mathbf{k} - \mathbf{k}'|, d)}{\epsilon(|\mathbf{k} - \mathbf{k}'|)} \right|^2 \frac{(1 + \cos \vartheta_{\mathbf{k}, \mathbf{k}'})}{2} \delta(\varepsilon_s(\mathbf{k}') - \varepsilon_{s'}(\mathbf{k})),$$

where

a) n_i is the number of impurities per unit area.

$$\text{b) } V_i(|\mathbf{k} - \mathbf{k}'|, d) = 2\pi e^2 \frac{\exp(-d|\mathbf{k} - \mathbf{k}'|)}{\tilde{\kappa} |\mathbf{k} - \mathbf{k}'|}$$

- d is the location of the charged impurity measured from the graphene sheet
- $\tilde{\kappa}$ is the effective dielectric constant, defined by $4\pi\epsilon_0 (\kappa_{top} + \kappa_{bottom}) / 2$, where ϵ_0 is the vacuum dielectric constant and κ_{top} and κ_{bottom} are the relative dielectric constants of the medium above and below the graphene layer.

$$\text{c) } \epsilon(|\mathbf{k} - \mathbf{k}'|) = \begin{cases} 1 + \frac{q_s}{|\mathbf{k} - \mathbf{k}'|} - \frac{\pi q_s}{8k_F} & \text{if } |\mathbf{k} - \mathbf{k}'| < 2k_F \\ 1 + \frac{q_s}{|\mathbf{k} - \mathbf{k}'|} - \frac{q_s \sqrt{|\mathbf{k} - \mathbf{k}'|^2 - 4k_F^2}}{2|\mathbf{k} - \mathbf{k}'|^2} - \frac{q_s}{4k_F} \text{asin} \left(\frac{2k_F}{|\mathbf{k} - \mathbf{k}'|} \right) & \text{otherwise} \end{cases}$$

is the 2D finite temperature static random phase approximation (RPA) dielectric (screening) function appropriate for graphene;

- $q_s = \frac{4e^2 k_F}{\tilde{\kappa} \hbar v_F}$ is the effective Thomas-Fermi wave-vector for graphene; it can be rewritten in terms of the dimensionless Wigner-Seitz radius r_s as $q_s = 4r_s k_F$;
- $k_F = \frac{\varepsilon_F}{\hbar v_F}$ is the Fermi wave-vector. We remark that if $\varepsilon_F = 0$ the dielectric function is not defined than according to [31] we adopt the approximate expression $k_F = \sqrt{\frac{4\pi n}{g_s g_v}}$, being n the 2D carrier density, $g_s = 2$ and $g_v = 2$ the spin and valley degeneracy. Hence the adopted threshold value in terms of Fermi level where the two expression switches is $|\varepsilon_F| = 0.04$ eV.

We remark that in (1.35), since the scattering is elastic and due to the presence of the delta function the only admissible cases are given by $s = s'$. The physical parameters adopted in our simulations are summarized in Table 1.2 and regard the silicon dioxide (SiO₂) and the hexagonal boron nitride (h-BN).

	SiO ₂	h-BN
$\hbar\omega_{op-ac}$	55 meV	200 meV
D_f	5.14×10^7 eV/cm	1.29×10^9 eV/cm
n_i	2.5×10^{11} cm ⁻²	2.5×10^{10} cm ⁻²
κ_{bottom}	3.9	3

TABLE 1.2: Physical parameters for the (el-sub) collision term.

1.3.3 Electron-electron interaction

The collision term including electron-electron interactions reads (see [101, 1]):

$$Q^{(el-el)}(f_s, f_{-s}) = \sum_{s'} \sum_{\mathbf{k}'_1, \mathbf{k}_2, \mathbf{k}'_2} [f_{s'}(\mathbf{k}'_1) f_{s'}(\mathbf{k}'_2) s_{ee}(\mathbf{k}'_1, \mathbf{k}'_2, \mathbf{k}_1, \mathbf{k}_2) (1 - f_s(\mathbf{k}_1)) (1 - f_s(\mathbf{k}_2)) + \\ - f_s(\mathbf{k}_1) f_s(\mathbf{k}_2) s_{ee}(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}'_1, \mathbf{k}'_2) (1 - f_{s'}(\mathbf{k}'_1)) (1 - f_{s'}(\mathbf{k}'_2))] ,$$

where the only dependence on $\mathbf{k}$ is written to avoid an annoying notation. $s_\alpha(\mathbf{k}, \mathbf{k}')$ is the transition rate from the state $\mathbf{k}$ to $\mathbf{k}'$ due to the interaction with the α th phonon branch while $s_{ee}(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}'_1, \mathbf{k}'_2)$ is the transition rate among the states $\mathbf{k}_1 \rightarrow \mathbf{k}'_1$ e $\mathbf{k}_2 \rightarrow \mathbf{k}'_2$.

Following [55], the transition rate s_{ee} , obtained by means of the Fermi golden rule, is given by

$$s_{ee}(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}'_1, \mathbf{k}'_2) = \frac{2\pi}{\hbar} |M|^2 \delta(\varepsilon(\mathbf{k}'_1) + \varepsilon(\mathbf{k}'_2) - \varepsilon(\mathbf{k}_1) - \varepsilon(\mathbf{k}_2)),$$

where the dispersion relation around the Dirac points of the first Brillouin zone is assumed to be $\varepsilon(\mathbf{k}) = \hbar v_F |\mathbf{k}|$. The generic element of the interaction matrix, is

$$|M|^2 = \frac{1}{2} \left[|V(q)|^2 + |V(q')|^2 - V(q)V(q') \right],$$

with

$$V(q) = \frac{2\pi e^2}{\epsilon(q)qA} \frac{1 + \cos(\phi_{\mathbf{k}_1, \mathbf{k}'_1})}{2} \frac{1 + \cos(\phi_{\mathbf{k}_2, \mathbf{k}'_2})}{2},$$

where $q = |\mathbf{k}_1 - \mathbf{k}'_1|$. In the above expressions $\phi_{\mathbf{k}, \mathbf{k}'}$ indicates the angle between $\mathbf{k}$ and $\mathbf{k}'$. For further details see [36], [93] e [14].

Under the hypothesis of *random-phase approximation* (valid for density $n \geq 10^{12} \text{cm}^{-2}$), the dielectric function $\epsilon(q)$ is given by ([34]):

$$\epsilon(q) = 1 + v_c(q)\Pi(q),$$

where $v_c(q) = 2\pi e^2 / \kappa q$, with κ (*background lattice dielectric constant*) which satisfies the relation $r_s = \frac{e^2}{\kappa \gamma} \sqrt{\frac{4}{g_s g_v}}$, Here $\gamma = \hbar v_F$, where g_s and g_v are the spin and valley degeneracy, and r_s a dimensionless constant (the *Wigner-Seitz radius*). If we introduce the function $\tilde{\Pi}(q) = \tilde{\Pi}^-(q) + \tilde{\Pi}^+(q)$, with

$$\tilde{\Pi}^-(q) = \frac{\pi q}{8k_F}$$

and

$$\tilde{\Pi}^+(q) = \begin{cases} 1 - \frac{\pi q}{8k_F} & \text{se } q < 2k_F \\ 1 - \frac{\sqrt{q^2 - 4k_F^2}}{2q} - \frac{q}{4k_F} \arcsin\left(\frac{2k_F}{q}\right) & \text{altrimenti} \end{cases},$$

where $k_F = \sqrt{4\pi n / g_s g_v}$, n being the electron density, one has $\Pi(q) = D(E_F)\tilde{\Pi}(q)$. $D(\varepsilon) = \frac{g_v g_s |\varepsilon|}{2\pi \gamma^2}$ is the density of state. A more detailed discussion about the physical aspects can be found in [19] e [31].

1.4 The drift-diffusion-Poisson model

The resolution of the semiclassical Boltzmann equation requires a huge computational effort. For that reason macroscopic models have been formulate. For graphene a hydrodynamical model based on the maximum entropy principle (MEP) has been formulated in [18] using a set of field variables which proved to be successful for traditional

semiconductors as silicon [69, 88, 87, 92, 91, 76, 66], gallium arsenide [69, 68], silicon carbide [2].

The drift-diffusion equations constitute a very popular model to describe semiconductor devices. The success of such a model is due to its practical use in engineering to design electronic devices. The drift-diffusion equations were first derived by van Roosbroeck in 1950 [90]. A derivation using a simple collision operator can be found in [49], while in [83] there was presented a rigorous derivation employing low-density operator. A result on existence and uniqueness of transient solutions can be found in [48]. In this section we describe the basics of the drift-diffusion model for graphene based electron devices.

1.4.1 The drift-diffusion equation

The bipolar drift-diffusion model for charge transport in graphene in the 1D case reads

$$\begin{aligned} \frac{\partial n}{\partial t} - \frac{1}{e} \frac{\partial}{\partial x} \left(\mu_n k_B T_L \frac{\partial n}{\partial x} - en \mu_n \frac{\partial \phi}{\partial x} \right) &= -R + G, \\ \frac{\partial p}{\partial t} + \frac{1}{e} \frac{\partial}{\partial x} \left(-\mu_p k_B T_L \frac{\partial p}{\partial x} - ep \mu_p \frac{\partial \phi}{\partial x} \right) &= -R + G, \end{aligned} \quad (1.36)$$

where $n(t, x)$, $p(t, x)$ are the graphene electron density and hole density respectively, e is the positive elementary charge, k_B is the Boltzmann constant, T_L is the lattice temperature (kept constant), $\mu_n(x)$ and $\mu_p(x)$ are the mobility models for electrons and holes respectively, $\phi(x, y)$ is the electric potential and R and G are the recombination and generation terms respectively.

The crucial issue is to devise appropriate models for the mobilities and the recombination-generation terms. A mobility model based on experimental data is presented in [33], while a new one based on numerical solutions of the semiclassical Boltzmann equation has been introduced in [62]. In [81] an improvement due to the bipolar charge transport including inter-band scatterings is presented. Finally in [79] the effects of the substrate where graphene is placed on are taken into account.

Usually the characteristic times of the recombination-generation terms are much longer than the typical evolution times. Moreover, for a Fermi energy greater than 0.2 eV, $R - G$ is essentially negligible because the Pauli exclusion principle prevents the formation of electron-hole couples. For a Fermi energy less than -0.2 eV practically there are not electrons around the Dirac point and again $R - G$ is essentially negligible [63].

1.4.2 The Poisson equation for the electric potential

In general the electric potential is coupled with the drift-diffusion equations by a 2D Poisson equation

$$\nabla \cdot (\epsilon \nabla \phi) = h(x, y), \quad (1.37)$$

where

$$h(x, y) = \begin{cases} e(n(x) - p(x))/t_{gr} & \text{if } y = y_{gr} \\ 0 & \text{if } y \neq y_{gr} \end{cases}$$

being y_{gr} the y -coordinate of the graphene sheet, t_{gr} the thickness of the graphene layer and ϵ is given by

$$\epsilon(x, y) = \begin{cases} \epsilon_{gr} & \text{if } y = y_{gr} \\ \epsilon_{ox} & \text{if } y \neq y_{gr} \end{cases}$$

where ϵ_{gr} and ϵ_{ox} are the dielectric constants of the graphene and oxide respectively.

The geometry of the problem depends on the particular device is taking into account. More details will be furnished in Chapter 4, where numerical simulation of a graphene based electron device will be showed.

Chapter 2

Numerical methods

A reasonable and physically accurate model for charge transport is based on semiclassical Boltzmann equations (quantum effects have also been included in the literature, e.g. see [6, 74]). Usually, the available solutions have been obtained by direct Monte Carlo simulations, e.g. a new Direct Simulation Monte Carlo (DSMC) procedure has been devised in [89, 25, 64] 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 [56] while a Discontinuous Galerkin (DG) method has been used in [89, 26, 62]. See [22, 21] for application of the DG method to traditional semiconductors, while numerical schemes for the Wigner equation can be found in [77].

On the other hand macroscopic models, such as drift-diffusion, have been formulated and frequently adopted in electronic engineering to simulate electron devices. A drift-diffusion model for graphene based electronics has been outlined in the previous chapter. To numerically solve it we adopt a strategy based on the Scharfetter-Gummel [94] scheme suitably adapted to the case under consideration. It belongs in the class of finite difference methods and furnishes a second order approximation in space and first order in time. For further details see [96].

This chapter is structured as follows: in Section 2.1 we devise the DG approach and in Section 2.2 we introduce the DSMC method both adopted for the solution of the semiclassical Boltzmann equation, in Section 2.3 we outline the finite difference approach for the numerical solution of the drift-diffusion system coupled with the Poisson equation.

2.1 The Discontinuous Galerkin method for treatment of the semiclassical Boltzmann equation

Discontinuous Galerkin (DG) methods are a class of finite element methods in which discontinuous basis functions, which are usually chosen as piecewise polynomials, are

used. Due to the above mentioned discontinuity, these methods presents many advantages: they can be used for arbitrary decomposition, in each element the polynomial degree can be chosen independent of that in the neighbors, to get the accuracy of the scheme elements only communicate with immediate neighbors [98].

The first DG method was introduced in 1973 to numerically solve the neutron transport equation [86]. A very important development consisted to get a general method to solve non-linear time-dependent problems using high order Runge–Kutta time discretizations and DG discretization in space with exact or approximate Riemann solvers as interface fluxes [23].

To get direct solutions of the semiclassical Boltzmann equation DG methods have been adopted by the applications to conventional semiconductors, like silicon [22, 21]. Recently this approach was extended to graphene to obtain numerical solutions of the spatially homogeneous Boltzmann equation for electrons in n-doped graphene both suspended [89] and on a substrate [25, 64]. Here a further extension to the bipolar case, contemplating intrinsic or low-doped situations, has been outlined first for suspended graphene [63] and also when it is placed on an oxide substrate [27]. In this section we are going to describe the DG method for the spatially homogeneous case (1.30).

2.1.1 Numerical discretization

Let us consider the bipolar semiclassical Boltzmann equation in the spatially homogeneous case,

$$\frac{\partial f_s}{\partial t} - \frac{e}{\hbar} \mathbf{E} \cdot \nabla_{\mathbf{k}} f_s = Q(f_s, f_{-s}) \quad (s = \pm 1), \quad (2.1)$$

where $f_s = f_s(t, \mathbf{k})$ represents the distribution function of charge carriers in the conduction band (CB), for $s = 1$, or in the valence band (VB), for $s = -1$, at time t and wave-vector $\mathbf{k} \in \mathbb{R}^2$.

Since we expect an exponential decay of f_+ and $1 - f_-$, as $|\mathbf{k}| \rightarrow +\infty$, it is reasonable to choose a compact domain $\Omega \subseteq \mathbb{R}^2$, such that $f_+(t, \mathbf{k}) \approx 0$ and $1 - f_-(t, \mathbf{k}) \approx 0$, for every $\mathbf{k} \notin \Omega$, and for every $\mathbf{x}$ and $t > 0$.

Now we introduce a finite decomposition $\{C_\alpha : \alpha = 1, 2, \dots, N\}$ of the domain Ω , with the C_α 's open sets such that

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

We assume a constant approximation for each distribution function f_s in every cell C_α . If we denote by χ_α the characteristic function relative to the cell C_α , then

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

A set of partial differential equations is now derived from the Boltzmann equations (1.28). The new unknowns are the $f_s^\alpha(\mathbf{t})$'s instead of the distribution functions $f_s(\mathbf{t}, \mathbf{k})$. Formally integrating Eq. (1.28) over each cell C_α , we obtain

$$\int_{C_\alpha} \frac{\partial f_s}{\partial t} d\mathbf{k} - \int_{C_\alpha} \frac{e}{\hbar} \mathbf{E} \cdot \nabla_{\mathbf{k}} f_s d\mathbf{k} = \int_{C_\alpha} Q(f_s, f_{-s}) d\mathbf{k}. \quad (2.2)$$

2.1.2 Numerical flux

The first integral of Eq. (2.2) can be approximated easily; in fact we have

$$\int_{C_\alpha} \frac{\partial f_s}{\partial t}(\mathbf{t}, \mathbf{k}) d\mathbf{k} \approx \text{meas}(C_\alpha) \frac{\partial f_s^\alpha}{\partial t}(\mathbf{t})$$

where $\text{meas}(C_\alpha)$ is the measure (area) of the cell C_α .

The integral involving the electric field is transformed by using the Gauss theorem,

$$-\frac{e}{\hbar} \mathbf{E} \cdot \int_{C_\alpha} \nabla_{\mathbf{k}} f_s d\mathbf{k} = -\frac{e}{\hbar} \mathbf{E} \cdot \int_{\partial C_\alpha} f_s \mathbf{n} d\sigma.$$

Since the approximation of f_s is not defined on the boundary of the cells, we must introduce a numerical flux, that furnishes reasonable values of f_s on every ∂C_α , depending on the values of the approximation of f_s in the nearest neighbors of the cell C_α and on the sign of $\mathbf{E} \cdot \mathbf{n}$. We have used a reconstruction of the fluxes based on a Min-Mod slope limiter, as in [25].

The numerical flux used is the *Min-Mod slope limiter*. The following is a description in a 1D case. We want to approximate the function $g(z)$ at the grid vertex $z_{n+\frac{1}{2}}$, known the averages of the cells centered at z_{n-1} , z_n , z_{n+1} and z_{n+2} . Fixed a wind velocity a

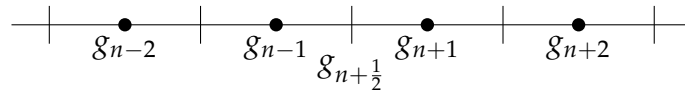


FIGURE 2.1: Stencil of the Min-Mod flux limiter in the 1D case.

and a spatial step Δz , the value of $g_{n+\frac{1}{2}}$ is

$$g_{n+\frac{1}{2}} \approx \begin{cases} g_n + \frac{\Delta z}{2} g'_n & \text{if } a > 0 \\ g_{n+1} + \frac{\Delta z}{2} g'_{n+1} & \text{if } a < 0 \end{cases}$$

where, for $a > 0$ (by instance), we have

$$g'_n \approx \begin{cases} \min\{|d_-|, |d_+|\} \operatorname{sgn}(d_-) & \text{if } d_- d_+ > 0 \\ 0 & \text{otherwise} \end{cases}$$

being

$$d_- = \frac{g_n - g_{n-1}}{\Delta z}, \quad d_+ = \frac{g_{n+1} - g_n}{\Delta z}.$$

For $a < 0$ a similar formula holds. This choice assures the second order in space [41].

We remark that the spatial gradient $\nabla_{\mathbf{x}} f_s(\mathbf{t}, \mathbf{x}, \mathbf{k})$ of (1.28) can be discretized in the same way as the drift one. In this case the discretization depends on the geometry of the spatial domain and boundary conditions (see for instance [22, 21]). Since in this paper we consider only space homogeneous solutions, the details are skipped.

2.1.3 Collision term

The treatment of the term arising from the collision operator is straightforward. If $\mathbf{k} \in C_\alpha$, then we have

$$\begin{aligned} Q(f_s, f_{-s}) &= \sum_{s'} \left[(1 - f_s(\mathbf{t}, \mathbf{k})) \int S_{s',s}(\mathbf{k}', \mathbf{k}) f_{s'}(\mathbf{t}, \mathbf{k}') d\mathbf{k}' \right. \\ &\quad \left. - f_s(\mathbf{t}, \mathbf{k}) \int S_{s,s'}(\mathbf{k}, \mathbf{k}') (1 - f_{s'}(\mathbf{t}, \mathbf{k}')) d\mathbf{k}' \right] \\ &\approx \sum_{s'} \sum_{\beta=1}^N \left[(1 - f_s^\alpha(\mathbf{t})) \int_{C_\beta} S_{s',s}(\mathbf{k}', \mathbf{k}) f_{s'}(\mathbf{t}, \mathbf{k}') d\mathbf{k}' \right. \\ &\quad \left. - f_s^\alpha(\mathbf{t}) \int_{C_\beta} S_{s,s'}(\mathbf{k}, \mathbf{k}') (1 - f_{s'}(\mathbf{t}, \mathbf{k}')) d\mathbf{k}' \right] \\ &\approx \sum_{s'} \sum_{\beta=1}^N \left[(1 - f_s^\alpha(\mathbf{t})) f_{s'}^\beta(\mathbf{t}) \int_{C_\beta} S_{s',s}(\mathbf{k}', \mathbf{k}) d\mathbf{k}' \right. \\ &\quad \left. - f_s^\alpha(\mathbf{t}) (1 - f_{s'}^\beta(\mathbf{t})) \int_{C_\beta} S_{s,s'}(\mathbf{k}, \mathbf{k}') d\mathbf{k}' \right]. \end{aligned}$$

So, defining

$$A_{s,s'}^{\alpha,\beta} = \int_{C_\alpha} \left[\int_{C_\beta} S_{s,s'}(\mathbf{k}, \mathbf{k}') d\mathbf{k}' \right] d\mathbf{k}, \quad (2.3)$$

it is immediate to verify that

$$\int_{C_\alpha} Q(f_s, f_{-s}) d\mathbf{k} \approx \sum_{s'} \sum_{\beta=1}^N \left[A_{s',s}^{\beta,\alpha} (1 - f_s^\alpha(t)) f_{s'}^\beta(t) - A_{s,s'}^{\alpha,\beta} f_s^\alpha(t) (1 - f_{s'}^\beta(t)) \right]. \quad (2.4)$$

In order to complete the numerical treatment of the Boltzmann equation it is necessary to specify the numerical domain in the $\mathbf{k}$ -space. We choose the circle $|\mathbf{k}| \leq k_{max}$, where k_{max} is a fixed maximum value such that f_+ and $1 - f_-$ are negligible for all $\mathbf{k}$ such that $|\mathbf{k}| > k_{max}$. The parameter k_{max} is checked a posteriori by means of numerical experiments.

We use modified polar coordinates by setting $\mathbf{k} = \sqrt{p}(\cos \vartheta, \sin \vartheta)$, and we introduce a regular decomposition (see Fig. 2.2). Hence the cell C_α is defined by the inequalities

$$0 \leq p_\alpha < p < p_\alpha + \Delta p \leq \sqrt{k_{max}} \quad \text{and} \quad 0 \leq \vartheta_\alpha < \vartheta < \vartheta_\alpha + \Delta \vartheta \leq 2\pi,$$

where Δp and $\Delta \vartheta$ are constant for every cell C_α .

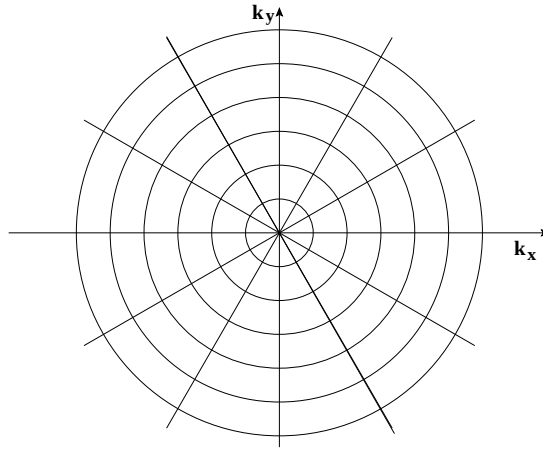


FIGURE 2.2: Grid in polar coordinates used for the discretization of the $\mathbf{k}$ -domain.

The use of the variable $\sqrt{p}$ instead of the modulus of $\mathbf{k}$ is aimed at having integrable parameters arising from the force term of the Boltzmann equation. Now, one can obtain the explicit expression of the numerical parameters $A_{s,s'}^{\alpha,\beta}$. Since the transition matrix

elements $|G_{s,s'}^{(\nu)}(\mathbf{k}, \mathbf{k}')|$ depend only on the convex angle between $\mathbf{k}$ and $\mathbf{k}'$, we can write

$$A_{s,s'}^{\alpha,\beta} = \frac{1}{4} \sum_{\nu} \Gamma_{s,s'}^{(\nu)}(\alpha, \beta) \int_{p_{\alpha}}^{p_{\alpha}+\Delta p} \int_{p_{\beta}}^{p_{\beta}+\Delta p} \left[(n_{\mathbf{q}}^{(\nu)} + 1) \delta(s' \hbar v_F \sqrt{p'} - s \hbar v_F \sqrt{p} + \hbar \omega_{\mathbf{q}}^{(\nu)}) + n_{\mathbf{q}}^{(\nu)} \delta(s' \hbar v_F \sqrt{p'} - s \hbar v_F \sqrt{p} - \hbar \omega_{\mathbf{q}}^{(\nu)}) \right] dp' dp, \quad (2.5)$$

where

$$\Gamma_{s,s'}^{(\nu)}(\alpha, \beta) = \int_{\vartheta_{\alpha}}^{\vartheta_{\alpha}+\Delta\vartheta} \int_{\vartheta_{\beta}}^{\vartheta_{\beta}+\Delta\vartheta} |G_{s,s'}^{(\nu)}(\mathbf{k}, \mathbf{k}')|^2 d\vartheta' d\vartheta. \quad (2.6)$$

The integrals in Eq. (2.6) are elementary. The integrals in Eq. (2.5) can be solved analytically, taking into account that

$$\begin{aligned} I(\alpha, \beta, s, s', \pm \omega_{\mathbf{q}}^{(\nu)}) &= \frac{1}{4} \int_{p_{\alpha}}^{p_{\alpha}+\Delta p} \int_{p_{\beta}}^{p_{\beta}+\Delta p} \delta(s' \hbar v_F \sqrt{p'} - s \hbar v_F \sqrt{p} \pm \hbar \omega_{\mathbf{q}}^{(\nu)}) dp' dp \\ &= \frac{1}{|s'| \hbar v_F} \int_{\sqrt{p_{\alpha}}}^{\sqrt{p_{\alpha}+\Delta p}} \int_{\sqrt{p_{\beta}}}^{\sqrt{p_{\beta}+\Delta p}} \delta\left(r' - \frac{s}{s'} r \pm \frac{\omega_{\mathbf{q}}^{(\nu)}}{s' v_F}\right) r r' dr' dr \\ &= \frac{1}{\hbar v_F} \int_{\sqrt{p_{\alpha}}}^{\sqrt{p_{\alpha}+\Delta p}} \left[\int_{\mathbb{R}} \chi_{[\sqrt{p_{\beta}}, \sqrt{p_{\beta}+\Delta p}]}(r') \delta\left(r' - \frac{s}{s'} r \pm \frac{\omega_{\mathbf{q}}^{(\nu)}}{s' v_F}\right) r' dr' \right] r dr \\ &= \frac{1}{\hbar v_F} \int_{\sqrt{p_{\alpha}}}^{\sqrt{p_{\alpha}+\Delta p}} \left(\frac{s}{s'} r \mp \frac{\omega_{\mathbf{q}}^{(\nu)}}{s' v_F} \right) \chi_{[\sqrt{p_{\beta}}, \sqrt{p_{\beta}+\Delta p}]} \left(\frac{s}{s'} r \mp \frac{\omega_{\mathbf{q}}^{(\nu)}}{s' v_F} \right) r dr, \end{aligned}$$

where $\chi_{[\sqrt{p_{\beta}}, \sqrt{p_{\beta}+\Delta p}]}$ is the characteristic function in the interval $[\sqrt{p_{\beta}}, \sqrt{p_{\beta}+\Delta p}]$. Now, we define the set

$$\left\{ r \in \mathbb{R} \text{ such that } \sqrt{p_{\alpha}} \leq r \leq \sqrt{p_{\alpha}+\Delta p} \text{ and } \sqrt{p_{\beta}} \leq \frac{s}{s'} r \mp \frac{\omega_{\mathbf{q}}^{(\nu)}}{s' v_F} \leq \sqrt{p_{\beta}+\Delta p} \right\},$$

which is the empty set or an interval $[a, b]$. In the first case the integral vanishes, and in the last case, we have

$$I(\alpha, \beta, s, s', \pm \omega_{\mathbf{q}}^{(\nu)}) = \frac{1}{\hbar v_F} \int_a^b \left(\frac{s}{s'} r^2 \mp \frac{\omega_{\mathbf{q}}^{(\nu)}}{s' v_F} r \right) dr,$$

that is an elementary integral. The integrals involving the electric field are derived by means of the same technique used in [25].

2.1.4 Macroscopic quantities

We observe that considering the distribution f_h of holes in the VB instead of the one of electrons, one gets that also $f_h \approx 0$ for all $\mathbf{k} \notin \Omega$, similarly to f_+ , and this helps the numerical approach that we use for the integration of the transport equations.

From the approximation of the distribution functions, the average values of density, velocity and energy are reconstructed as follows

$$\begin{aligned}
\rho_e(t) &:= \frac{2}{(2\pi)^2} \int f_+(t, \mathbf{k}) d\mathbf{k} \approx \frac{2}{(2\pi)^2} \sum_{\alpha=1}^N \text{meas}(C_\alpha) f_+^\alpha(t), \\
\langle \mathbf{v}_e \rangle(t) &:= \frac{1}{\rho_e(t)} \frac{2}{(2\pi)^2} \int f_+(t, \mathbf{k}) \mathbf{v}_+(\mathbf{k}) d\mathbf{k} \\
&\approx \frac{1}{\rho_e(t)} \frac{2}{(2\pi)^2} \sum_{\alpha=1}^N \left[\int_{C_\alpha} \mathbf{v}_+(\mathbf{k}) d\mathbf{k} \right] f_+^\alpha(t), \\
\langle \varepsilon_e \rangle(t) &:= \frac{1}{\rho_e(t)} \frac{2}{(2\pi)^2} \int f_+(t, \mathbf{k}) \varepsilon_+(\mathbf{k}) d\mathbf{k} \\
&\approx \frac{1}{\rho_e(t, \mathbf{x})} \frac{2}{(2\pi)^2} \sum_{\alpha=1}^N \left[\int_{C_\alpha} \varepsilon_+(\mathbf{k}) d\mathbf{k} \right] f_+^\alpha(t), \\
\rho_h(t) &:= \frac{2}{(2\pi)^2} \int (1 - f_-(t, -\mathbf{k})) d\mathbf{k} \approx \frac{2}{(2\pi)^2} \sum_{\alpha=1}^N \text{meas}(C_\alpha) (1 - f_-^\alpha(t)), \\
\langle \mathbf{v}_h \rangle(t) &:= \frac{1}{\rho_h(t)} \frac{2}{(2\pi)^2} \int f_h(t, \mathbf{k}) \mathbf{v}_h(\mathbf{k}) d\mathbf{k} \\
&= \frac{1}{\rho_h(t)} \frac{2}{(2\pi)^2} \int (1 - f_-(t, -\mathbf{k})) \mathbf{v}_h(\mathbf{k}) d\mathbf{k} \\
&= \frac{1}{\rho_h(t)} \frac{2}{(2\pi)^2} \int (1 - f_-(t, -\mathbf{k})) \mathbf{v}_+(\mathbf{k}) d\mathbf{k} \\
&\approx -\frac{1}{\rho_h(t)} \frac{2}{(2\pi)^2} \sum_{\alpha=1}^N \left[\int_{C_\alpha} \mathbf{v}_+(\mathbf{k}) d\mathbf{k} \right] (1 - f_-^\alpha(t)), \\
\langle \varepsilon_h \rangle(t) &:= \frac{1}{\rho_h(t)} \frac{2}{(2\pi)^2} \int (1 - f_-(t, -\mathbf{k})) \varepsilon_+(\mathbf{k}) d\mathbf{k} \\
&\approx \frac{1}{\rho_h(t)} \frac{2}{(2\pi)^2} \sum_{\alpha=1}^N \left[\int_{C_\alpha} \varepsilon_+(\mathbf{k}) d\mathbf{k} \right] (1 - f_-^\alpha(t)).
\end{aligned}$$

The above integrals are easily evaluated by taking into account that

$$\begin{aligned} \text{meas}(C_\alpha) &= \frac{1}{2} \Delta p \Delta \vartheta, \\ \int_{C_\alpha} \mathbf{v}_s d\mathbf{k} &= s v_F \Delta p \left(\cos\left(\vartheta + \frac{\Delta \vartheta}{2}\right) \sin \frac{\Delta \vartheta}{2}, \sin\left(\vartheta + \frac{\Delta \vartheta}{2}\right) \sin \frac{\Delta \vartheta}{2} \right), \\ \int_{C_\alpha} \varepsilon_s(\mathbf{k}) d\mathbf{k} &= \frac{1}{3} s v_F \hbar \Delta \vartheta \left[\sqrt{(p_\alpha + \Delta p)^3} - \sqrt{(p_\alpha)^3} \right]. \end{aligned}$$

Regarding the current density $\mathbf{J}$, it is given by the sum of the contribution from electrons in the CB and holes in the VB

$$\mathbf{J} = \mathbf{J}_e + \mathbf{J}_h.$$

The term $\mathbf{J}_e$ is given by $-e\rho_e \langle \mathbf{v}_e \rangle$ while

$$\mathbf{J}_h = e \frac{2}{(2\pi)^2} \int (1 - f_-(t, -\mathbf{k})) \mathbf{v}_h(\mathbf{k}) d\mathbf{k} = -e \frac{2}{(2\pi)^2} \int (1 - f_-(t, \mathbf{k})) \mathbf{v}_h(\mathbf{k}) d\mathbf{k}.$$

2.2 The Direct Simulation Monte Carlo approach to numerically solve the semiclassical Boltzmann equation

To numerically solve the Boltzmann equation an important role is played by stochastic simulations. Monte Carlo methods identify a group of techniques using random variables, artificially generated by a computer, to solve mathematical problems. The name Monte Carlo appeared the first time in a paper written by N.C. Metropolis and S. Ulam in 1949 [71]. Direct Simulation Monte Carlo method is referred to a numerical probabilistic Monte Carlo technique to model rarefied gas flows. It was introduced the first time by G.A. Bird in 1970 [12]. Thirty years later it was proved that DSMC converges to the solution of the Boltzmann equation [104]. About the charge transport, DSMC simulates the dynamics of charge carriers inside the crystal. The approach is described in [46, 44].

A crucial point is the correct inclusion of the Pauli Exclusion Principle (PEP). The approach proposed in [60] allows an occupation number greater than one with an evident violation of PEP. About the simulation of charge transport in graphene, in [89] a new approach is employed. It predicts occupation numbers consistent with PEP and therefore is physically more accurate. Moreover, in presence of an oxide substrate where graphene is placed on, scatterings with remote impurities are treated in [25] and [24]. Furthermore, thermal effects are also taken into account in [26, 30].

In this section we are going to describe the adopted DSMC algorithm for the semiclassical Boltzmann equation for electrons in CB where electron-phonon and electron-substrate interactions are taken into account.

2.2.1 Numerical settings

The $\mathbf{k}$ -space is approximated by the set $[-k_{x\max}, k_{x\max}] \times [-k_{y\max}, k_{y\max}]$ with $k_{x\max}$ and $k_{y\max}$ such that the number of electrons with a wave-vector $\mathbf{k}$ outside such a set is practically negligible. The $\mathbf{k}$ -space is partitioned into a uniform rectangular grid. We shall denote by C_{ij} the generic cell of the grid centered at the $\mathbf{k}_{ij}$ wave-vector.

The distribution function is approximated with a piecewise constant function in each cell. At time $t = 0$ the n_p particles used for the simulation are distributed in each cell according to the equilibrium Fermi-Dirac distribution.

The maximum number n_{ij}^* of simulated particles accommodated in each cell is easily evaluated (see [60]). Let N_{ij} be the number of real particles in the cell C_{ij} and let n_{ij} be the number of simulated particles in the same cell. Let A be the area of the sample and let N be the number of real particles in the sample, $N = \rho A$. By observing that N/n_p is the statistical weight of each particle entering the simulation and taking into account the condition $0 \leq f \leq 1$, one has

$$\begin{aligned} n_{ij} &= \frac{N_{ij}}{N} n_p = \frac{n_p}{N} \frac{2}{(2\pi)^2} A \int_{C_{ij}} f d\mathbf{k} \leq \frac{n_p}{N} \frac{2}{(2\pi)^2} A \int_{C_{ij}} d\mathbf{k} \\ &= \frac{2}{(2\pi)^2} \text{meas}(C_{ij}) \frac{n_p}{N} A = \frac{2}{(2\pi)^2} \text{meas}(C_{ij}) \frac{n_p}{\rho} = n_{ij}^*, \end{aligned} \quad (2.7)$$

where $\text{meas}(C_{ij})$ is the measure of the cell C_{ij} . Of course n_{ij}^* is not in general an integer, therefore rounding errors are introduced. Usually the problem is solved by using a number of simulated particles n_p great enough to make such errors negligible. The convergence of the procedure is often checked just by comparing the results with different n_p .

2.2.2 The DSMC method

In the standard approach the motion of each particles is described alternating free-flight, that is governed by the semiclassical equation of motion

$$\hbar \dot{\mathbf{k}} = -e \mathbf{E}, \quad (2.8)$$

and scattering, that changes the wavevector of particles according to the collision term.

The main concern with the procedure delineated above is that, according to the semiclassical approximation, the compatibility with Pauli's exclusion principle of the positions occupied during the free flight is not checked. *It may occur that the particle at the end of the free-flight reaches a cell in the $\mathbf{k}$ -space already fully occupied making the occupation number greater than one* (see [89]).

It is of course nonphysical the fact that, for high values of the Fermi energy, the maximum occupation number can greatly exceed the maximum one, although the average quantities could be acceptable according to the law of large numbers. Even if the scattering can redistribute the particles among the cells, in general it is not possible to eliminate the presence of anomalous occupation numbers.

For overcoming the problem, in [100] it has been proposed to apply the rejection technique not only to the scattering events but also at the end of each free-flight. However, even implementing this variant, the same drawbacks are still present as shown in [89].

In order to avoid such a difficulty, in [89] the following approach has been proposed. The crucial point in the previous procedure is the step concerning the free-flight. If we go back to the original transport equation, we can use a splitting scheme to avoid nonphysical results. The basic idea is to reformulate the splitting method in terms of a particle method.

In a time interval Δt , first we solve the drift part of the equation corresponding to the free-flight in the analogous DSMC approach,

$$\frac{\partial f(t, \mathbf{k})}{\partial t} - \frac{e}{\hbar} \mathbf{E} \cdot \nabla_{\mathbf{k}} f(t, \mathbf{k}) = 0, \quad (2.9)$$

taking as initial condition the distribution at time t , and then the collision part

$$\frac{\partial f(t, \mathbf{k})}{\partial t} = Q(f)(t, \mathbf{k}), \quad (2.10)$$

taking as initial condition the solution of Eq. (2.9).

The collision term is the most involved and delicate part and it is particularly important to include PEP to describe charge transport in graphene correctly. This implies a heavy computational cost and requires an update of the distribution function at each time step.

Now we describe the numerical scheme for the electron-phonon and electron-substrate collision term. The time interval Δt is chosen for each particle in a random way by means of

$$\Delta t = -\frac{\ln \xi}{\Gamma_{tot}(\varepsilon(t))}, \quad (2.11)$$

where ξ is a random number with uniform distribution in the interval $[0, 1]$ and Γ_{tot} being the total scattering rate of the particle, having energy ε at time t .

$$\Gamma_{tot}(\varepsilon(t)) = \sum_v \Gamma_v(\varepsilon(t)) + \Gamma_{ss}(\varepsilon(t)).$$

The generic scattering rate Γ_v is defined by

$$\Gamma_v(\mathbf{k}) = \int_{\mathbb{R}^2} S^{(v)}(\mathbf{k}, \mathbf{k}') d\mathbf{k}'$$

depending on $\mathbf{k}$ through the energy, that is $\Gamma_v(\mathbf{k}) = \Gamma_v(\varepsilon)$. The symbol v identifies the scattering type, ac, TO, K, for the electron-phonon collision term and TO-sub, imp for the electron-substrate collision term. The function Γ_{ss} , called *self-scattering rate*, is the scattering rate associated to a fictitious scattering that does not change the state of the electron. The self-scattering rate is determined by considering the sum $\Gamma_M = \sum_v \Gamma_v$. Hence Γ_{ss} is fixed in such a way $\Gamma_{tot} = \alpha \Gamma_M$, where $\alpha > 1$ is a tuning parameter. We set $\alpha = 1.1$ in our simulations. This method differs from the standard one (see for instance [45]).

The scattering is selected randomly according to the values of the transition rates, and PEP is taken into account as in [60]. Once the state after the scattering has been determined, denoted by $\mathbf{k}'$ its wave-vector, the initial state is changed or left the same according to the rejection technique. It consists to choose a random number ξ generated uniformly in $[0, 1]$ and, if $\xi < 1 - f(\mathbf{k}')$ the transition is accepted, otherwise it is rejected. Then, according to the angular distribution of the scattering rate, a rejection method allows to select the angular dependence of the wave-vector after the scattering event.

At fixed times the momentum, velocity, energy of each electron are stored and the mean values are evaluated in order to follow the time evolution of the system.

The global procedure gives a numerical approximation of $f(t + \Delta t, \mathbf{x}, \mathbf{k})$ up to first order in Δt . The solution of Eq. (2.9) is just a *rigid* translation of the distribution function along the characteristics and can be reformulated from a particle point of view as a free-flight of the same time step for each electron. In this way, the cells in the $\mathbf{k}$ -space are moved of the displacement vector $\hbar \Delta \mathbf{k} = -e \mathbf{E} \Delta t$ but without changing the occupation number of the cells themselves. To avoid considering a computational domain too large, we adopt a Lagrangian approach and move the grid by adapting it to the new position of the cells, instead of moving the cells themselves.

Eq. (2.10) is solved by a sequence of collision steps for each particle during the time interval $[t, t + \Delta t]$ in a standard way. Since the collision mechanisms take into account PEP, the occupation number cannot exceed the maximum occupation number

in this second step as well. Hence, neither the drift nor the collision step give rise to the possibility of having, in a single cell, more particles than the maximum occupation number.

The overall scheme is a hybrid approach which furnishes a first order in time approximation of the distribution function. Average quantities can be evaluated as well by taking the mean values of the quantities of interest, e.g. velocity and energy.

2.3 Finite difference method for the drift-diffusion-Poisson system

The drift-diffusion system (1.36), which forms the basic semiconductor equations, together with appropriate boundary conditions cannot be solved explicitly in general. Therefore, the solution must be calculated by means of numerical approaches.

The most successfully adopted are the *finite difference method*, the *finite box method* which indeed is just a more general finite difference method and the *finite element method* [96].

2.3.1 Discretization of the drift-diffusion system

Let us consider the one dimensional drift-diffusion equations (1.36) and introduce a uniform mesh of N_x grid points and size Δx in the simulation space interval $[x_2, x_3]$ along with a constant time step Δt . The numerical approximation of a generic function $u(x, t)$ at the node j and time $k\Delta t$ will be denoted by u_j^k .

By introducing the Slotboom variables

$$s_n = n \exp(-\phi/U_T), \quad s_p = p \exp(\phi/U_T)$$

and by observing that

$$\frac{\partial s_n}{\partial x} = \frac{\partial n}{\partial x} \exp(-\phi/U_T) - \frac{n}{U_T} \exp(-\phi/U_T) \frac{\partial \phi}{\partial x} = \frac{\exp(-\phi/U_T)}{U_T} \left(U_T \frac{\partial n}{\partial x} - n \frac{\partial \phi}{\partial x} \right),$$

$$\frac{\partial s_p}{\partial x} = \frac{\partial p}{\partial x} \exp(\phi/U_T) + \frac{p}{U_T} \exp(\phi/U_T) \frac{\partial \phi}{\partial x} = \frac{\exp(\phi/U_T)}{U_T} \left(U_T \frac{\partial p}{\partial x} + p \frac{\partial \phi}{\partial x} \right),$$

one can put the current the currents in the following form

$$\begin{aligned} J_n &= e\mu_n U_T \exp(\phi/U_T) \frac{\partial s_n}{\partial x}, \\ J_p &= -e\mu_p U_T \exp(-\phi/U_T) \frac{\partial s_p}{\partial x}. \end{aligned}$$

Let us rewrite the previous relations as follows

$$\begin{aligned} e\mu_n U_T \frac{\partial s_n}{\partial x} &= J_n \exp(-\phi/U_T), \\ e\mu_p U_T \frac{\partial s_p}{\partial x} &= -J_p \exp(\phi/U_T). \end{aligned} \tag{2.12}$$

In each interval $[x_i, x_{i+1}]$ we suppose that the mobilities and the currents are constants, that is $\forall x \in [x_i, x_{i+1}]$

$$\mu_n(x) \approx \mu_{i+\frac{1}{2}}^n, \quad \mu_p(x) \approx \mu_{i+\frac{1}{2}}^p, \quad J_n(x) \approx J_{i+\frac{1}{2}}^n, \quad J_p(x) \approx J_{i+\frac{1}{2}}^p,$$

while we approximate ϕ in $[x_i, x_{i+1}]$ by a piecewise linear function

$$\phi(x) \approx \phi_i + \frac{x - x_i}{\Delta x} (\phi_{i+1} - \phi_i).$$

By integrating equations (2.12) in $[x_i, x_{i+1}]$ one obtains

$$e\mu_{i+\frac{1}{2}}^n U_T \int_{x_i}^{x_{i+1}} \frac{\partial s_n}{\partial x} dx = J_{i+\frac{1}{2}}^n \int_{x_i}^{x_{i+1}} \exp \left\{ -\frac{1}{U_T} \left[\phi_i + \frac{x - x_i}{\Delta x} (\phi_{i+1} - \phi_i) \right] \right\} dx$$

wherefrom

$$\begin{aligned} e\mu_{i+\frac{1}{2}}^n U_T (s_{i+1}^n - s_i^n) &= -\frac{U_T \Delta x}{\phi_{i+1} - \phi_i} J_{i+\frac{1}{2}}^n \left[\exp \left\{ -\frac{1}{U_T} \left[\phi_i + \frac{x - x_i}{\Delta x} (\phi_{i+1} - \phi_i) \right] \right\} \right]_{x_i}^{x_{i+1}} \\ &= -\frac{U_T \Delta x}{\phi_{i+1} - \phi_i} J_{i+\frac{1}{2}}^n [\exp(-\phi_{i+1}/U_T) - \exp(-\phi_i/U_T)]. \end{aligned}$$

which gives the following expression of $J_{i+\frac{1}{2}}^n$

$$\begin{aligned} J_{i+\frac{1}{2}}^n &= -e\mu_{i+\frac{1}{2}}^n \frac{\phi_{i+1} - \phi_i}{\Delta x} \frac{s_{i+1}^n - s_i^n}{\exp(-\phi_{i+1}/U_T) - \exp(-\phi_i/U_T)} \\ &= -e\mu_{i+\frac{1}{2}}^n \frac{\phi_{i+1} - \phi_i}{\Delta x} \frac{n_{i+1} \exp(-(\phi_{i+1} - \phi_i)/2U_T) - n_i \exp((\phi_{i+1} - \phi_i)/2U_T)}{\exp(-(\phi_{i+1} - \phi_i)/2U_T) - \exp((\phi_{i+1} - \phi_i)/2U_T)}. \end{aligned}$$

By setting

$$\sigma_{i+\frac{1}{2}} = \frac{\phi_{i+1} - \phi_i}{2},$$

the electron current can be rewritten in a compact form

$$\begin{aligned}
J_{i+\frac{1}{2}}^n &= e \frac{\mu_{i+\frac{1}{2}}^n}{\Delta x} \sigma_{i+\frac{1}{2}} \frac{2n_{i+1} \exp(-\sigma_{i+\frac{1}{2}}/U_T) - 2n_i \exp(\sigma_{i+\frac{1}{2}}/U_T)}{\exp(\sigma_{i+\frac{1}{2}}/U_T) - \exp(-\sigma_{i+\frac{1}{2}}/U_T)} \\
&= e \frac{\mu_{i+\frac{1}{2}}^n}{\Delta x} \frac{\sigma_{i+\frac{1}{2}}}{\exp(\sigma_{i+\frac{1}{2}}/U_T) - \exp(-\sigma_{i+\frac{1}{2}}/U_T)} \\
&\quad \cdot \left\{ n_{i+1} \left[\exp(\sigma_{i+\frac{1}{2}}/U_T) + 2 \exp(-\sigma_{i+\frac{1}{2}}/U_T) - \exp(\sigma_{i+\frac{1}{2}}/U_T) \right] \right. \\
&\quad \left. - n_i \left[\exp(-\sigma_{i+\frac{1}{2}}/U_T) + 2 \exp(\sigma_{i+\frac{1}{2}}/U_T) - \exp(-\sigma_{i+\frac{1}{2}}/U_T) \right] \right\} \\
&= e \frac{\mu_{i+\frac{1}{2}}^n}{\Delta x} \sigma_{i+\frac{1}{2}} \left[(n_{i+1} - n_i) \frac{\exp(\sigma_{i+\frac{1}{2}}/U_T) + \exp(-\sigma_{i+\frac{1}{2}}/U_T)}{\exp(\sigma_{i+\frac{1}{2}}/U_T) - \exp(-\sigma_{i+\frac{1}{2}}/U_T)} \right. \\
&\quad \left. + (n_{i+1} + n_i) \frac{\exp(-\sigma_{i+\frac{1}{2}}/U_T) - \exp(\sigma_{i+\frac{1}{2}}/U_T)}{\exp(\sigma_{i+\frac{1}{2}}/U_T) - \exp(-\sigma_{i+\frac{1}{2}}/U_T)} \right] \\
&= e \frac{\mu_{i+\frac{1}{2}}^n}{\Delta x} \sigma_{i+\frac{1}{2}} \left[(n_{i+1} - n_i) \coth(\sigma_{i+\frac{1}{2}}/U_T) - (n_{i+1} + n_i) \right].
\end{aligned}$$

Similarly for the hole current we find

$$J_{i+\frac{1}{2}}^p = -e \frac{\mu_{i+\frac{1}{2}}^p}{\Delta x} \sigma_{i+\frac{1}{2}} \left[(p_{i+1} - p_i) \coth(\sigma_{i+\frac{1}{2}}/U_T) + (p_{i+1} + p_i) \right].$$

We discretize equations (1.36) with respect to time by the forward Euler scheme and with respect to space, in the interior grid points, by central finite differences

$$\begin{aligned}
\frac{n_i^{k+1} - n_i^k}{\Delta t} - \frac{1}{e} \frac{\left(J_{i+\frac{1}{2}}^n \right)^k - \left(J_{i-\frac{1}{2}}^n \right)^k}{\Delta x} &= 0 \\
\frac{p_i^{k+1} - p_i^k}{\Delta t} + \frac{1}{e} \frac{\left(J_{i+\frac{1}{2}}^p \right)^k - \left(J_{i-\frac{1}{2}}^p \right)^k}{\Delta x} &= 0
\end{aligned}$$

for $i = 2, \dots, N_x - 1$. Then, by substituting the previous expressions of the current, the explicit scheme for the densities is obtained

$$\begin{aligned}
n_i^{k+1} &= n_i^k + \frac{\Delta t}{\Delta x^2} \left\{ \mu_{i+\frac{1}{2}}^n \sigma_{i+\frac{1}{2}} \left[(n_{i+1}^k - n_i^k) \coth(\sigma_{i+\frac{1}{2}}/U_T) - (n_{i+1}^k + n_i^k) \right] \right. \\
&\quad \left. - \mu_{i-\frac{1}{2}}^n \sigma_{i-\frac{1}{2}} \left[(n_i^k - n_{i-1}^k) \coth(\sigma_{i-\frac{1}{2}}/U_T) - (n_i^k + n_{i-1}^k) \right] \right\}, \tag{2.13}
\end{aligned}$$

$$p_i^{k+1} = p_i^k - \frac{\Delta t}{\Delta x^2} \left\{ \mu_{i+\frac{1}{2}}^p \sigma_{i+\frac{1}{2}} \left[(p_{i+1}^k - p_i^k) \coth(\sigma_{i+\frac{1}{2}}/U_T) + (p_{i+1}^k + p_i^k) \right] \right. \\ \left. - \mu_{i-\frac{1}{2}}^p \sigma_{i-\frac{1}{2}} \left[(p_i^k - p_{i-1}^k) \coth(\sigma_{i-\frac{1}{2}}/U_T) + (p_i^k + p_{i-1}^k) \right] \right\}. \quad (2.14)$$

The variable without temporal index must be considered evaluated at the time step k .

2.3.2 Numerical discretization for the Poisson equation

To solve the Poisson equation (1.37) numerically a uniform two-dimensional mesh is adopted with mesh size along the y direction Δy while the mesh size along the x direction is still Δx , the same used for the equations (1.36). Moreover the graphene layer lies on a row of the 2D mesh. The Poisson equation is discretized by finite differences at the internal points with the standard five point stencil

$$\frac{\left(\varepsilon \frac{\partial \phi}{\partial x}\right)_{i+\frac{1}{2}} - \left(\varepsilon \frac{\partial \phi}{\partial x}\right)_{i-\frac{1}{2}}}{\Delta x} + \frac{\left(\varepsilon \frac{\partial \phi}{\partial y}\right)_{j+\frac{1}{2}} - \left(\varepsilon \frac{\partial \phi}{\partial y}\right)_{j-\frac{1}{2}}}{\Delta y} = h_{i,j},$$

for all $i = 2, \dots, N_x - 1$ and $j = 2, \dots, N_y - 1$, where N_y is the number of grid point in the y direction which depends on the x variable according to the geometry of the device, and

$$\begin{aligned} \left(\varepsilon \frac{\partial \phi}{\partial x}\right)_{i+\frac{1}{2}} &= \varepsilon_{i+\frac{1}{2},j} \frac{\phi_{i+1,j} - \phi_{i,j}}{\Delta x}, \\ \left(\varepsilon \frac{\partial \phi}{\partial x}\right)_{i-\frac{1}{2}} &= \varepsilon_{i-\frac{1}{2},j} \frac{\phi_{i,j} - \phi_{i-1,j}}{\Delta x}, \\ \left(\varepsilon \frac{\partial \phi}{\partial y}\right)_{j+\frac{1}{2}} &= \varepsilon_{i,j+\frac{1}{2}} \frac{\phi_{i,j+1} - \phi_{i,j}}{\Delta y}, \\ \left(\varepsilon \frac{\partial \phi}{\partial y}\right)_{j-\frac{1}{2}} &= \varepsilon_{i,j-\frac{1}{2}} \frac{\phi_{i,j} - \phi_{i,j-1}}{\Delta y}. \end{aligned}$$

The overall second order discretization is obtained

$$\begin{aligned} &\frac{\varepsilon_{i+\frac{1}{2},j} \phi_{i+1,j} - (\varepsilon_{i+\frac{1}{2},j} + \varepsilon_{i-\frac{1}{2},j}) \phi_{i,j} + \varepsilon_{i-\frac{1}{2},j} \phi_{i-1,j}}{\Delta x^2} \\ &+ \frac{\varepsilon_{i,j+\frac{1}{2}} \phi_{i,j+1} - (\varepsilon_{i,j+\frac{1}{2}} + \varepsilon_{i,j-\frac{1}{2}}) \phi_{i,j} + \varepsilon_{i,j-\frac{1}{2}} \phi_{i,j-1}}{\Delta y^2} = h_{i,j} \end{aligned}$$

The scheme is completed with appropriate boundary conditions.

Chapter 3

Bipolar charge transport in monolayer graphene

Charge transport in monolayer graphene is simulated by a numerical deterministic approach, based on a discontinuous Galerkin (DG) method, for solving the semiclassical Boltzmann equation for electrons. Both the conduction and valence bands are included and the interband scatterings are taken into account.

The use of a Direct Simulation Monte Carlo (DSMC) approach, which properly describes the interband scatterings, is computationally very expensive because the valence band is very populated and a huge number of particles is needed. Also the choice of simulating holes instead of electrons does not overcome the problem because there is a certain degree of ambiguity in the generation and recombination terms of electron-hole pairs. Often, direct solutions of the Boltzmann equations with a DSMC neglect the interband scatterings on the basis of physical arguments. The DG approach does not suffer from the previous drawbacks and requires a reasonable computing effort.

In the following chapter the importance of the interband scatterings is accurately evaluated for several values of the Fermi energy, addressing the issue related to the validity of neglecting the generation-recombination terms. Both the cases of suspended graphene and that one of graphene placed on a substrate are investigated. It is found out that the inclusion of the interband scatterings produces huge variations in the average values, as the current, with zero Fermi energy while, as expected, the effect of the interband scattering becomes negligible by increasing the absolute value of the Fermi energy.

We remark that the contents of this chapter are original and presented in Ref.s [63, 27].

3.1 Holes description

In general both electrons in the conduction and valence bands contribute to charge transport in graphene and the zero gap energy band allows for the creation of electron-hole pairs by scattering with phonons around the Dirac points. Therefore, one has also to include interband electron-phonon scatterings. However, if a gate voltage is applied, it is possible to modify the value of the Fermi energy ε_F creating a kind of doping as in conventional semiconductors. If ε_F is positive and high enough, one has a kind of n -doping and the only relevant contribution to the current is due to the electrons in the conduction band. Analogously, if $\varepsilon_F < 0$ one has a kind of p -doping. The use of DSMC in the bipolar case is rather heavy from a computational point of view because the valence band is very populated and a huge number of simulation particles are needed. A viable way to overcome the problem could be to simulate, in the valence band, holes instead of electrons. Unfortunately, this introduces a certain degree of ambiguity in the generation and recombination terms of electron-hole pairs and makes the approach rather questionable, as explained in the next section. For such a reason, often the interband scattering is neglected. The DG method does not suffer from the previous difficulties and keeps the computational effort to a reasonable level. In the present paper, by performing an extensive numerical simulation with the DG method of the system of Boltzmann equations for electrons in the conduction and valence bands, the importance of the interband scatterings is accurately evaluated for several values of the Fermi energy in the case of suspended monolayer graphene under a constant external electric field. It is addressed the issue related to the validity of neglecting the generation-recombination terms. It is found out that the inclusion of the interband scatterings induces huge variations in the average values, as the current, with zero Fermi energy while, as expected, the effect of the interband scatterings becomes negligible by increasing in absolute value the Fermi energy.

3.1.1 Deduction of the Boltzmann equation for holes

Starting from the Boltzmann equation for the distribution function of electrons in VB f_- one has

$$\partial_t f_-(t, \mathbf{x}, \mathbf{k}) + \mathbf{v}_-(\mathbf{k}) \cdot \nabla_{\mathbf{x}} f_-(t, \mathbf{x}, \mathbf{k}) - \frac{e}{\hbar} \mathbf{E} \cdot \nabla_{\mathbf{k}} f_-(t, \mathbf{x}, \mathbf{k}) = Q(f_-, f_+)(t, \mathbf{x}, \mathbf{k}), \quad (3.1)$$

where

$$\mathbf{v}_-(\mathbf{k}) = \frac{1}{\hbar} \nabla_{\mathbf{k}} \varepsilon_-(\mathbf{k}) = -\frac{1}{\hbar} \hbar v_F \nabla_{\mathbf{k}} |\mathbf{k}| = -v_F \frac{\mathbf{k}}{|\mathbf{k}|}$$

and

$$Q(f_-, f_+) = \int_{\mathbb{R}^2} [S_{-,-}(\mathbf{k}', \mathbf{k}) f_-(\mathbf{k}') (1 - f_-(\mathbf{k})) - S_{-,-}(\mathbf{k}, \mathbf{k}') f_-(\mathbf{k}) (1 - f_-(\mathbf{k}'))] d\mathbf{k}' \\ + \int_{\mathbb{R}^2} [S_{+,-}(\mathbf{k}', \mathbf{k}) f_+(\mathbf{k}') (1 - f_-(\mathbf{k})) - S_{+,-}(\mathbf{k}, \mathbf{k}') f_-(\mathbf{k}) (1 - f_+(\mathbf{k}'))] d\mathbf{k}'.$$

We would like to get the distribution of missing electron states, that are the holes. For these quasi-particles the following definitions hold

$$\mathbf{k}_h = -\mathbf{k}_e, \quad \varepsilon_h(\mathbf{k}_h) = -\varepsilon_-(\mathbf{k}_e).$$

Thus the dispersion relation and the distribution function for holes can be written respectively as

$$\varepsilon_h(\mathbf{k}) = \hbar v_F |\mathbf{k}|, \quad f_h(t, \mathbf{x}, \mathbf{k}) = 1 - f_-(t, \mathbf{x}, \mathbf{k}),$$

and the group velocity is

$$\mathbf{v}_h(\mathbf{k}) = \frac{1}{\hbar} \nabla_{\mathbf{k}} \varepsilon_h(\mathbf{k}) = v_F \frac{\mathbf{k}}{|\mathbf{k}|}.$$

Relabeling the variable $\mathbf{k}$ of equation (3.1) with $-\mathbf{k}$, the Boltzmann equation for the distribution function of missing electrons is

$$\partial_t (1 - f_-(t, \mathbf{x}, -\mathbf{k})) + \mathbf{v}_-(-\mathbf{k}) \cdot \nabla_{\mathbf{x}} (1 - f_-(t, \mathbf{x}, -\mathbf{k})) - \frac{e}{\hbar} \mathbf{E} \cdot \nabla_{-\mathbf{k}} (1 - f_-(t, \mathbf{x}, -\mathbf{k})) \\ = -Q(f_-, f_+)(t, \mathbf{x}, -\mathbf{k}).$$

After observing that

$$\mathbf{v}_-(-\mathbf{k}) = -v_F \frac{-\mathbf{k}}{|-\mathbf{k}|} = \mathbf{v}_h(\mathbf{k}),$$

we have

$$\partial_t f_h(t, \mathbf{x}, \mathbf{k}) + \mathbf{v}_h(\mathbf{k}) \cdot \nabla_{\mathbf{x}} f_h(t, \mathbf{x}, \mathbf{k}) + \frac{e}{\hbar} \mathbf{E} \cdot \nabla_{\mathbf{k}} f_h(t, \mathbf{x}, \mathbf{k}) = -Q(f_-, f_+)(t, \mathbf{x}, -\mathbf{k}).$$

Regarding the collisional term, we have

$$\begin{aligned}
-Q(f_-, f_+)(t, \mathbf{x}, -\mathbf{k}) &= \\
&= - \int_{\mathbb{R}^2} [S_{-,-}(\mathbf{k}', -\mathbf{k}) f_-(\mathbf{k}') (1 - f_-(-\mathbf{k})) - S_{-,-}(-\mathbf{k}, \mathbf{k}') f_-(-\mathbf{k}) (1 - f_-(\mathbf{k}'))] d\mathbf{k}' \\
&\quad - \int_{\mathbb{R}^2} [S_{+,-}(\mathbf{k}', -\mathbf{k}) f_+(\mathbf{k}') (1 - f_-(-\mathbf{k})) - S_{+,-}(-\mathbf{k}, \mathbf{k}') f_-(-\mathbf{k}) (1 - f_+(\mathbf{k}'))] d\mathbf{k}' \\
&= - \int_{\mathbb{R}^2} [S_{-,-}(\mathbf{k}', -\mathbf{k}) (1 - f_h(-\mathbf{k}')) f_h(\mathbf{k}) - S_{-,-}(-\mathbf{k}, \mathbf{k}') (1 - f_h(\mathbf{k})) f_h(-\mathbf{k}')] d\mathbf{k}' \\
&\quad - \int_{\mathbb{R}^2} [S_{+,-}(\mathbf{k}', -\mathbf{k}) f_+(\mathbf{k}') f_h(\mathbf{k}) - S_{+,-}(-\mathbf{k}, \mathbf{k}') (1 - f_h(\mathbf{k})) (1 - f_+(\mathbf{k}'))] d\mathbf{k}' \\
&= - \int_{\mathbb{R}^2} [S_{-,-}(-\mathbf{k}', -\mathbf{k}) f_h(\mathbf{k}) (1 - f_h(\mathbf{k}')) - S_{-,-}(-\mathbf{k}, -\mathbf{k}') f_h(\mathbf{k}') (1 - f_h(\mathbf{k}))] d\mathbf{k}' \\
&\quad - \int_{\mathbb{R}^2} [S_{+,-}(\mathbf{k}', -\mathbf{k}) f_+(\mathbf{k}') f_h(\mathbf{k}) - S_{+,-}(-\mathbf{k}, \mathbf{k}') (1 - f_h(\mathbf{k})) (1 - f_+(\mathbf{k}'))] d\mathbf{k}',
\end{aligned}$$

where the last step is obtained by performing a change of variables $\mathbf{k}' \rightarrow -\mathbf{k}'$. Definitely the collisional term writes

$$-Q(f_-, f_+)(t, \mathbf{x}, -\mathbf{k}) = Q_{hh}(f_h, f_h)(t, \mathbf{x}, \mathbf{k}) + Q_{he}(f_h, f_+)(t, \mathbf{x}, \mathbf{k}),$$

where, omitting the dependencies on t and $\mathbf{x}$,

$$\begin{aligned}
Q_{hh} &= - \int_{\mathbb{R}^2} [S_{-,-}(-\mathbf{k}', -\mathbf{k}) f_h(\mathbf{k}) (1 - f_h(\mathbf{k}')) - S_{-,-}(-\mathbf{k}, -\mathbf{k}') f_h(\mathbf{k}') (1 - f_h(\mathbf{k}))] d\mathbf{k}', \\
Q_{he} &= - \int_{\mathbb{R}^2} [S_{+,-}(\mathbf{k}', -\mathbf{k}) f_+(\mathbf{k}') f_h(\mathbf{k}) - S_{+,-}(-\mathbf{k}, \mathbf{k}') (1 - f_h(\mathbf{k})) (1 - f_+(\mathbf{k}'))] d\mathbf{k}'.
\end{aligned}$$

Let us consider the particular case where only intraband transitions are taken into account. The equation writes

$$\partial_t f_h(t, \mathbf{x}, \mathbf{k}) + \mathbf{v}_h(\mathbf{k}) \cdot \nabla_{\mathbf{x}} f_h(t, \mathbf{x}, \mathbf{k}) + \frac{e}{\hbar} \mathbf{E} \cdot \nabla_{\mathbf{k}} f_h(t, \mathbf{x}, \mathbf{k}) = Q_{hh}(t, \mathbf{x}, \mathbf{k}). \quad (3.2)$$

It is possible to prove that $S_{-,-}(-\mathbf{k}', -\mathbf{k}) = S_{-,-}(\mathbf{k}', \mathbf{k})$ by using geometrical considerations on the involved angles and, therefore, the relation $S_{-,-}(\mathbf{k}', \mathbf{k}) = S_{+,+}(\mathbf{k}, \mathbf{k}')$ holds.

Summarizing, the distribution function of holes $f_h(t, \mathbf{x}, \mathbf{k})$ satisfies the Boltzmann type equation

$$\partial_t f_h(t, \mathbf{x}, \mathbf{k}) + \mathbf{v}_h(\mathbf{k}) \cdot \nabla_{\mathbf{x}} f_h(t, \mathbf{x}, \mathbf{k}) + \frac{e}{\hbar} \mathbf{E} \cdot \nabla_{\mathbf{k}} f_h(t, \mathbf{x}, \mathbf{k}) = Q_h(f_h, f_+)(t, \mathbf{x}, \mathbf{k}),$$

where $\mathbf{v}_h$ is the group velocity of holes, that it can be shown to take the expression

$$\mathbf{v}_h(\mathbf{k}) = \frac{1}{\hbar} \nabla_{\mathbf{k}} \varepsilon_h(\mathbf{k}),$$

and Q_h is the collisional term for holes, which splits into

$$Q_h(f_h, f_+) = Q_{hh}(f_h, f_h) + Q_{he}(f_h, f_+). \quad (3.3)$$

Here (by omitting the explicit dependence on t and $\mathbf{x}$)

$$Q_{hh} = - \int_{\mathbb{R}^2} [S_{-,-}(-\mathbf{k}', -\mathbf{k}) f_h(\mathbf{k})(1 - f_h(\mathbf{k}')) - S_{-,-}(-\mathbf{k}, -\mathbf{k}') f_h(\mathbf{k}')(1 - f_h(\mathbf{k}))] d\mathbf{k}'$$

gives the intraband hole interactions (with phonons), while

$$Q_{he} = - \int_{\mathbb{R}^2} [S_{+,-}(\mathbf{k}', -\mathbf{k}) f_+(\mathbf{k}') f_h(\mathbf{k}) - S_{-,+}(-\mathbf{k}, \mathbf{k}')(1 - f_h(\mathbf{k}))(1 - f_+(\mathbf{k}'))] d\mathbf{k}'$$

represents the interband scatterings (with phonons).

At the equilibrium the distribution function of electrons in both bands is the Fermi-Dirac distribution, given by

$$f_{FD}^{\pm}(t, \mathbf{x}, \mathbf{k}) = \frac{1}{1 + \exp\left(\frac{\varepsilon_{\pm} - \varepsilon_F}{k_B T}\right)},$$

where ε_F is the Fermi energy and the sign $\pm$ indicates the CB (+) or the VB (-). Therefore, the equilibrium distribution of holes is given by

$$f_{FD}^h(t, \mathbf{x}, \mathbf{k}) = 1 - f_{FD}^-(t, \mathbf{x}, -\mathbf{k}) = 1 - \frac{1}{1 + \exp\left(\frac{\varepsilon_- - \varepsilon_F}{k_B T}\right)} = \frac{1}{1 + \exp\left(\frac{\varepsilon_h + \varepsilon_F}{k_B T}\right)}, \quad \varepsilon_h > 0,$$

that goes to 0 when $\varepsilon_h \mapsto +\infty$. We remark that, instead, $f_{FD}^- \mapsto 1$ when $\varepsilon_- \mapsto -\infty$.

3.1.2 Possibility to adopt a DSMC approach

If we take into account only intraband transitions, the equations are uncoupled, that is each particle belongs to the same population during the simulation. On the contrary, if we have also interband transitions it can happen for a particle to change energy band and thus population.

In the first case a DSMC algorithm can be construct by solving two Boltzmann equations: one for electrons in CB and one for holes in VB. In particular, the following relations

$$S_{-,-}(-\mathbf{k}', -\mathbf{k}) = S_{-,-}(\mathbf{k}', \mathbf{k}) = S_{+,+}(\mathbf{k}, \mathbf{k}') \quad (3.4)$$

hold.

Thus, the Boltzmann equation for holes in VB, in the case when only intraband transitions occur, is the same of that of electrons in CB, except for the sign in front of the elementary charge.

The fact that the valence band is populated with a huge number of electrons (recall that $f_- \approx 1$ when $|\mathbf{k}| \gg 1$), requires in a DSMC the introduction of a prohibitive number of particles. To overcome the problem one can consider holes in the valence band. However, such a choice has the drawback to make ambiguous the interband scattering mechanism, as explained below.

Let us consider an electron having energy ε . If it happens that $0 < \varepsilon < \hbar\omega^{(\nu)}$ and an emission of a ν th phonon occurs, where ν is OP or K, then an interband scattering event takes place. After the transition the electron will have a state determined according to the ν th transition rate (see [89]) and the new energy.

If we try to rewrite this interband scattering in terms of holes, instead of electrons, in the valence band, then the electron recombines with a hole. In order to have a recombination we need to find a hole having exactly the energy $\hbar\omega^{(\nu)} - \varepsilon$ and this can be achieved only in an approximate, often roughly, way.

The treatment of the case when a hole has an energy $0 < \varepsilon < \hbar\omega^{(\nu)}$ is even worse. After the scattering event the considered hole can disappear through two different mechanisms: an electron coming from the conduction band recombines with a hole or an electron of the valence band occupies the position of the hole leaving behind an other hole. The only viable approach to discriminate between the two occurrences is to describe both electrons and holes in the valence band and again we have to face the question related to the huge number of required simulation particles.

A similar ambiguity arises for the description of electron-hole pair creation.

The above considerations clearly indicate that the deterministic methods, as the DG adopted in [63, 27], are the only reasonable ones for solving the transport equations for charge carriers in graphene in the presence of interband scatterings.

3.2 Numerical results for suspended case

The physical situation we are going to 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. 3.1). This allows us to look for solutions which are not depending on space and to avoid any effect related to the boundary conditions.

We have considered several values of the Fermi energy and different applied electric fields.

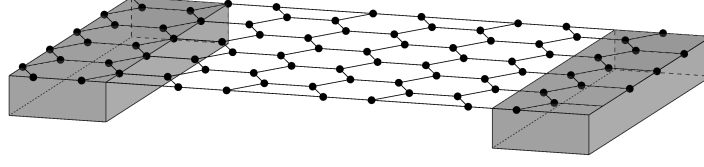


FIGURE 3.1: Schematic representation of a suspended monolayer graphene. In the direction parallel to the contacts the material is infinitely long. In each contact there is a constant electrostatic potential.

Case $\varepsilon_F = 0$ eV

This case represents a pristine graphene and it is the most challenging for the correct evaluation of the role of the interband scattering. In Fig.3.2 there is shown the density versus time (in logarithmic scale). During a long transient of a few hundreds of picoseconds, the concentration of both charge carriers increases up to saturation values depending on the applied electric field. The effect is that of carrier multiplications and it is due to the fact that the generation term overcomes for a long time that of recombination with the results of the creation of electron-hole pairs. Only after about 200 picosecond the conduction band is populated enough so that Pauli's exclusion principle becomes so efficient to prevent the formation of additional electron-hole pairs. A similar phenomenon had have been observed for example in [85] and in [107] analyzing the optical properties of graphene in view of possible applications to solar cells. We remark that when $\varepsilon_F = 0$ eV, the electron and hole densities are the same. For this reason only the electron density is plotted. Of course, neglecting the interband scatterings, the densities do not change with time. For comparison, also the densities without interband scattering are reported in the figures.

In Fig.3.3 the total current (electrons plus holes) is plotted versus time. Similarly to the density, the current increases with time, apart an initial transient. The carrier multiplication leads to a considerably higher current with respect to the case when only intraband scatterings are included. The steady total current versus the electric field is reported in Fig.3.4. Note that neglecting the interband scatterings introduces an error of about 400% for the highest electric field considered in the simulation (10 kV/cm).

Case $\varepsilon_F = 0.1$ eV

In order to assess the influence of the Fermi level, the case with $\varepsilon_F = 0.1$ eV has been also analyzed. The results are shown in Fig.s 3.5,3.6,3.7. First we note that the electron and hole densities are no longer equal. Moreover, as expected, the difference is about two orders of magnitude because electrons are the majority carriers when the Fermi

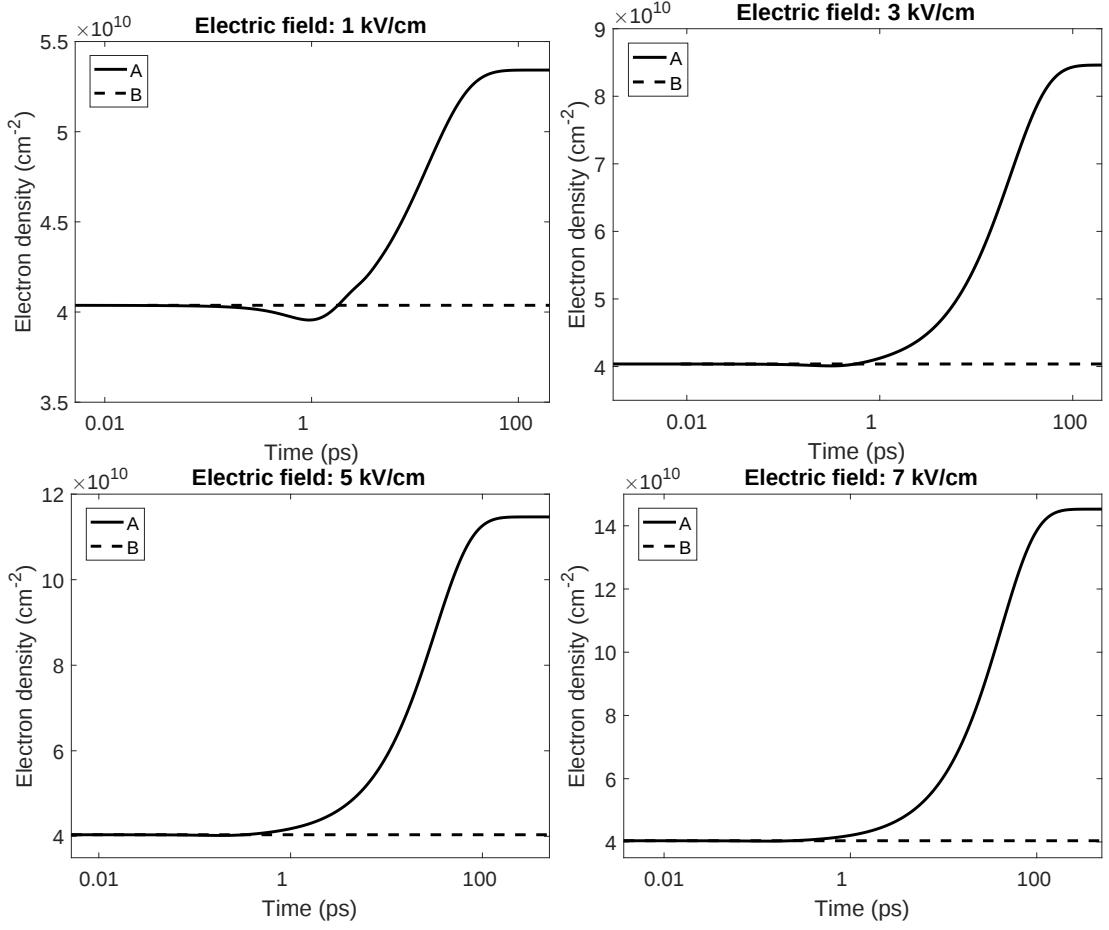


FIGURE 3.2: Electron density versus time when $\varepsilon_F = 0$ eV under an applied electric field of 1, 3, 5, 7 kV/cm with (A) and without (B) interband scatterings.

energy is positive. The maximum change obtained in the simulations with respect to the case without interband scatterings is less than 1% for electrons and more than 90% for holes. This means that neglecting the interband effects leads to severely underestimate the hole density. Regarding the discrepancy in the current, for the electric field of 10 kV/cm one has a relative difference of about 22%.

If the reverse sign of Fermi energy is considered, we have the same results by interchanging the role of electrons and holes.

Case $\varepsilon_F = 0.2$ eV

Finally, the case with $\varepsilon_F = 0.2$ eV has been analyzed. The results are shown in Figs 3.8, 3.9, 3.10. The transient is shorter: the Pauli exclusion principle drastically reduces the formation of electron-hole pairs already after few picoseconds. The electron density remains practically unchanged, while that of holes increases more than one order of magnitude. However, the difference between the majority and minority charges

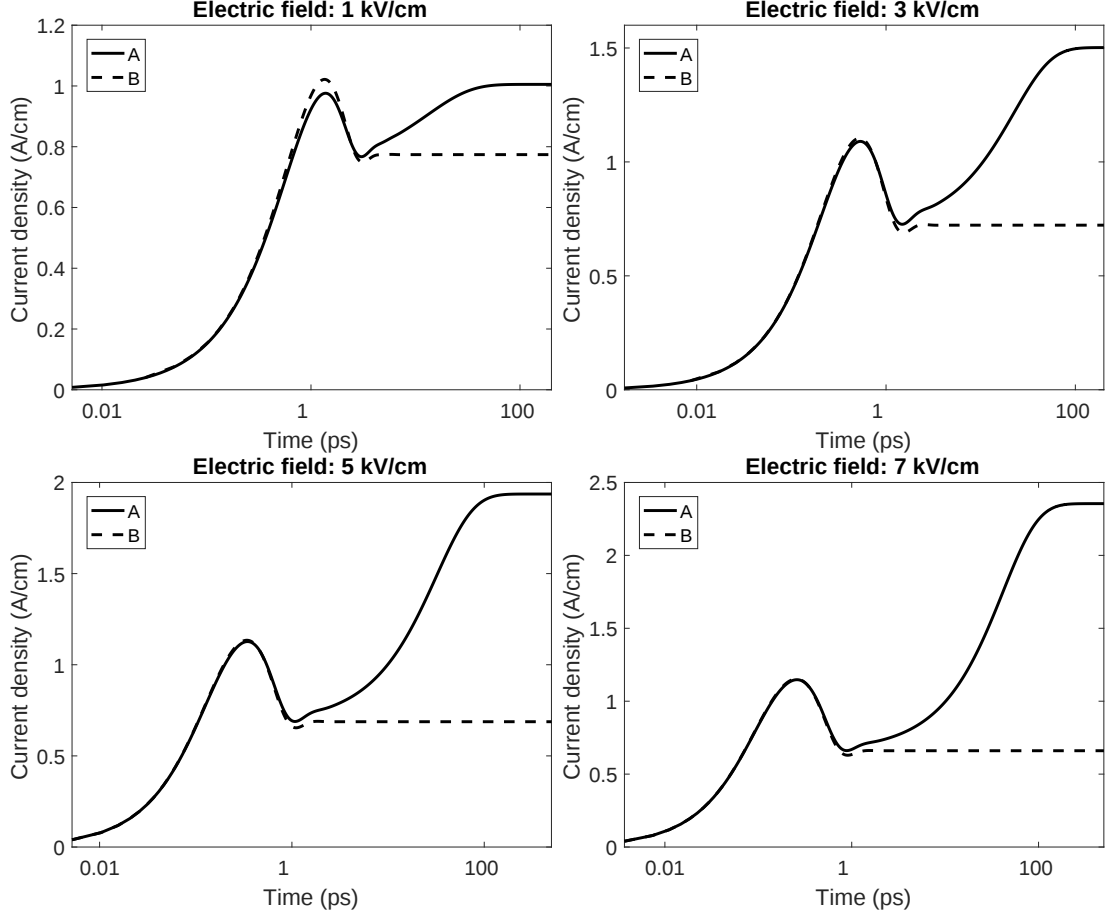


FIGURE 3.3: Total current versus time when $\varepsilon_F = 0$ eV under an applied electric field of 1, 3, 5, 7 kV/cm with (A) and without (B) interband scatterings.

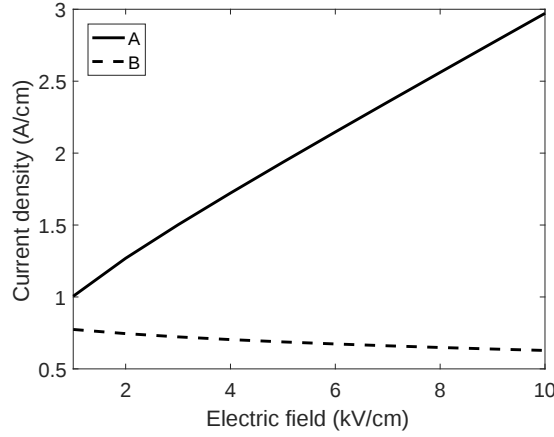


FIGURE 3.4: Steady total current versus electric field when $\varepsilon_F = 0$ eV with (A) and without (B) interband scatterings.

is so high that, for Fermi levels greater or equal to 0.2 eV, the simulation can be performed with a good accuracy disregarding the interband effects. If the reverse sign of Fermi energy is considered, we have again the same results by interchanging the role

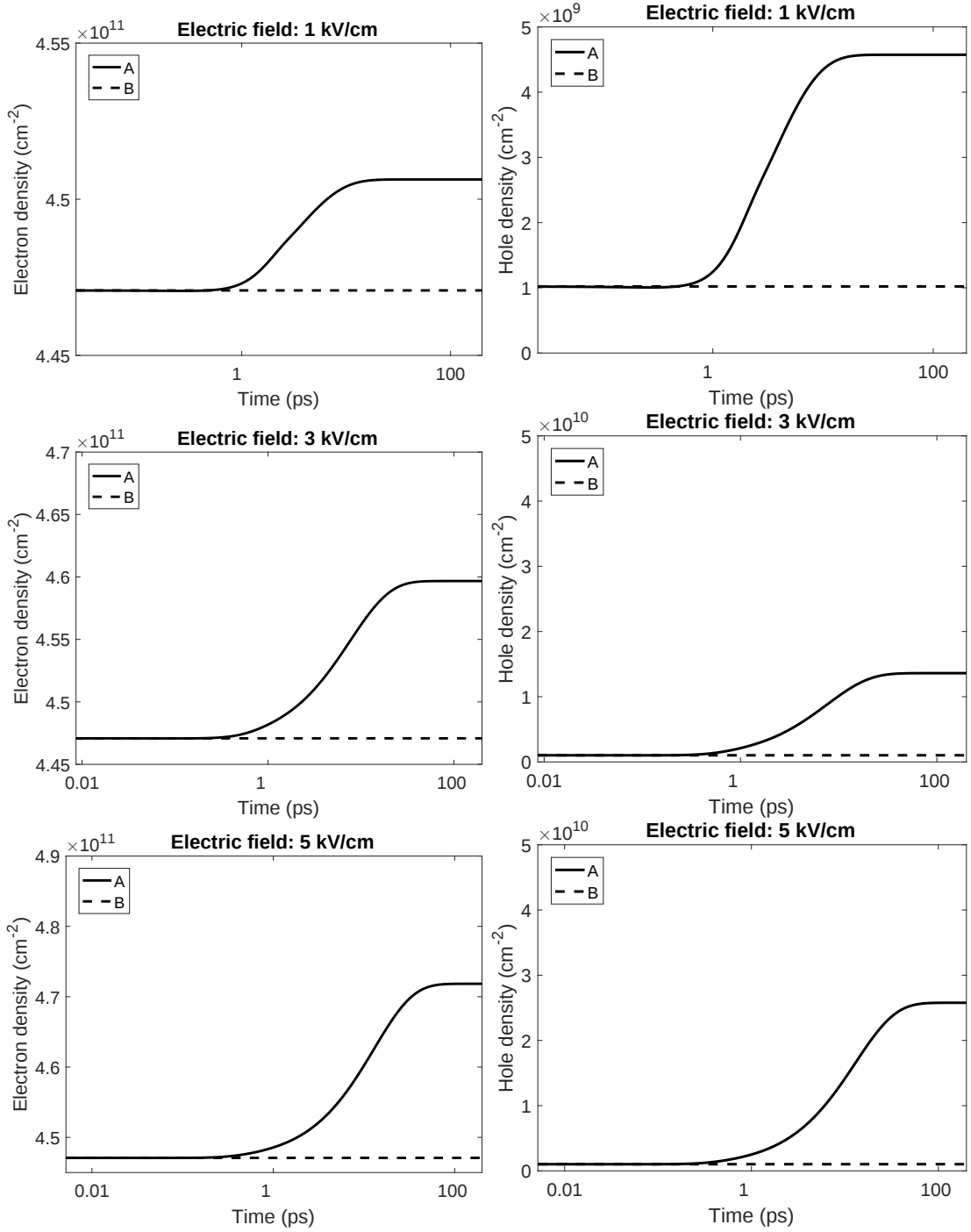


FIGURE 3.5: Electron density (left column) and hole density (right column) versus time when $\varepsilon_F = 0.1$ eV under an applied field of 1, 3, 5 kV/cm with (A) and without (B) interband scatterings.

of electrons and holes.

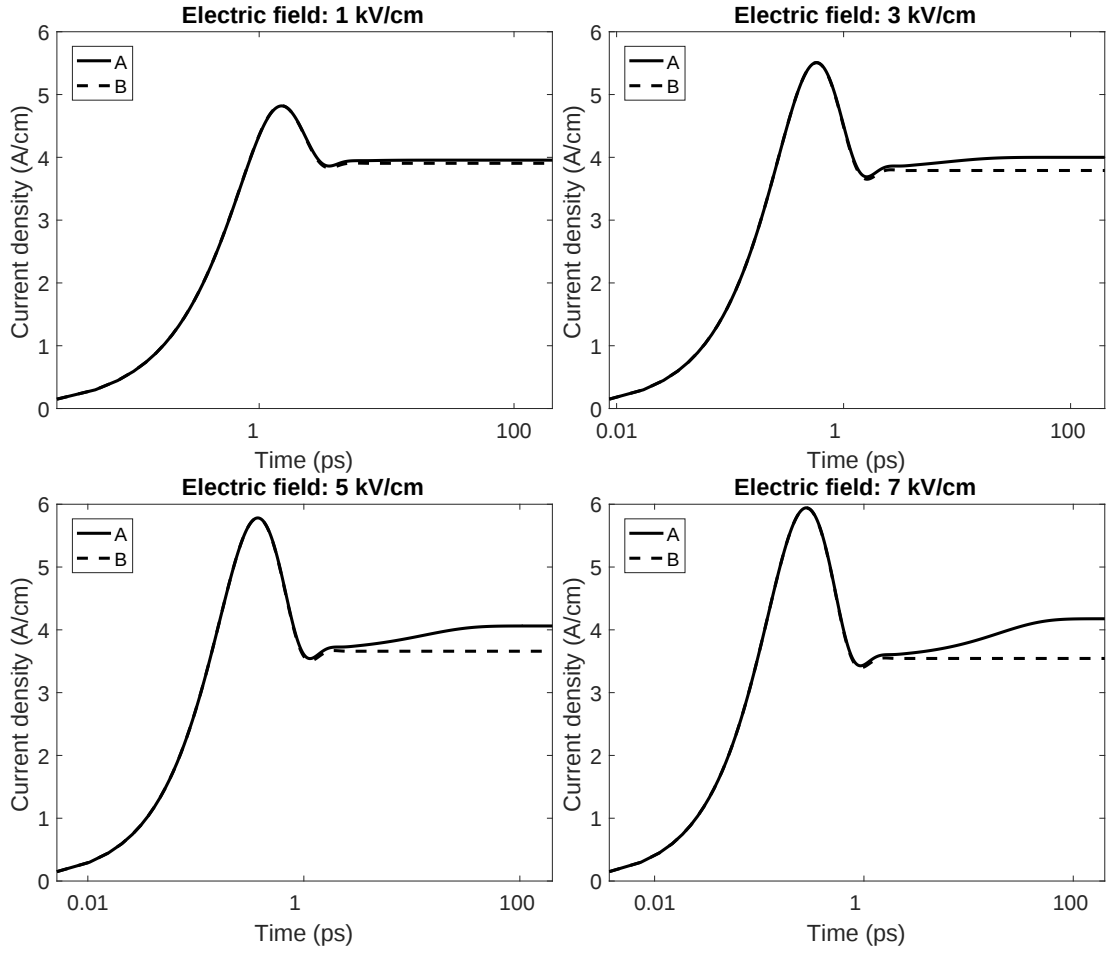


FIGURE 3.6: Total current versus time when $\varepsilon_F = 0.1$ eV under an applied electric field of 1, 3, 5, 7 kV/cm with (A) and without (B) interband scatterings.

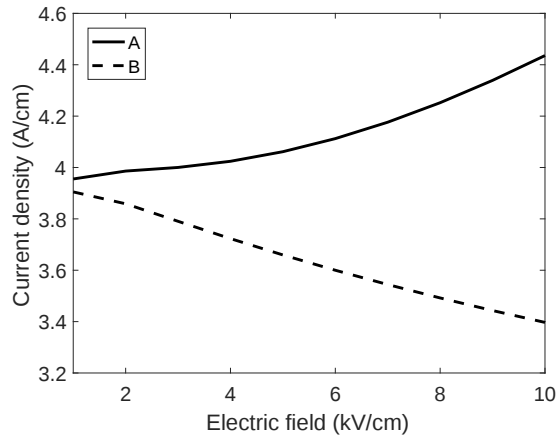


FIGURE 3.7: Steady total current versus electric field when $\varepsilon_F = 0.1$ eV.

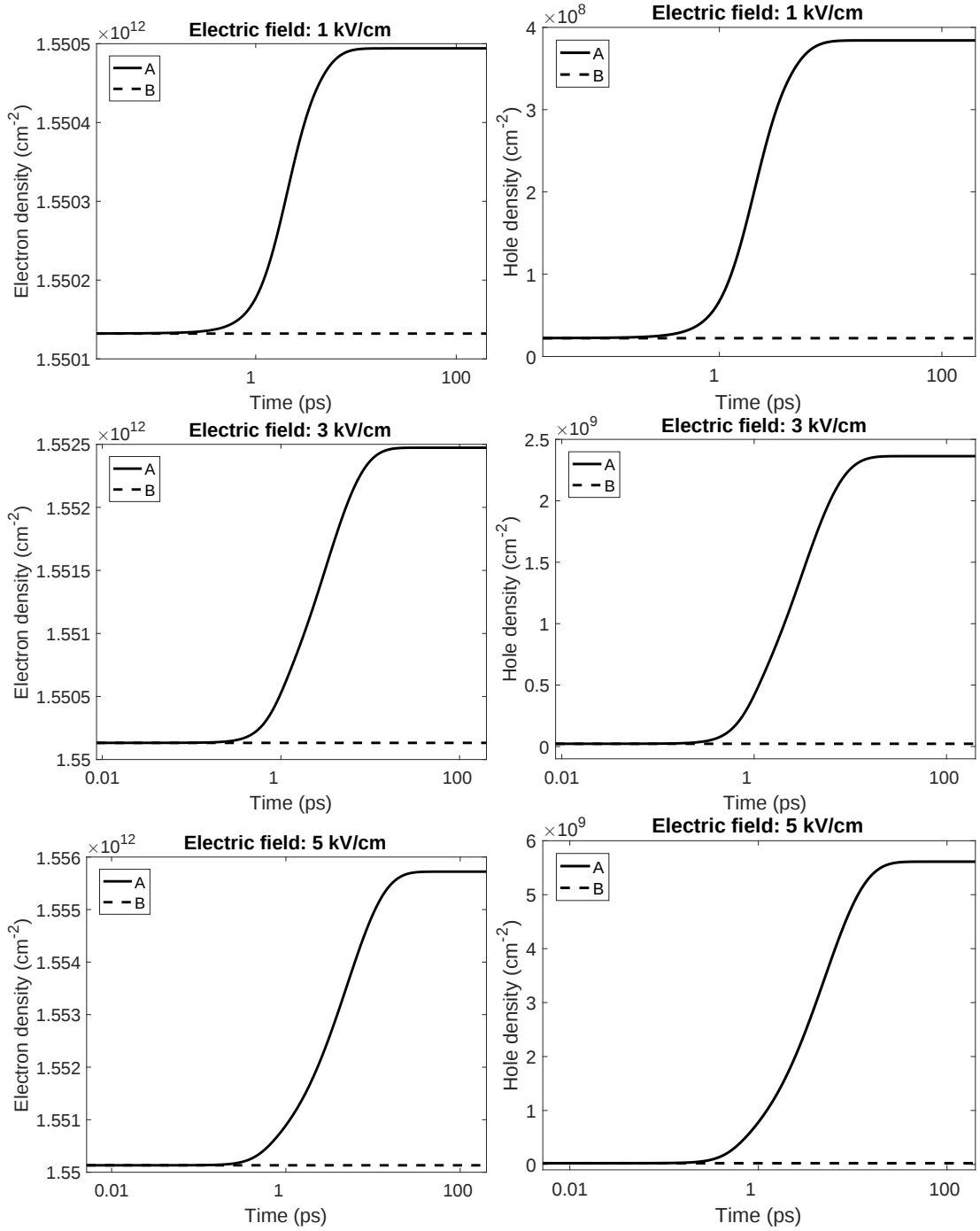


FIGURE 3.8: Electron density (left column) and hole density (right column) versus time when $\varepsilon_F = 0.2$ eV under an applied electric field of 1, 3, 5 kV/cm.

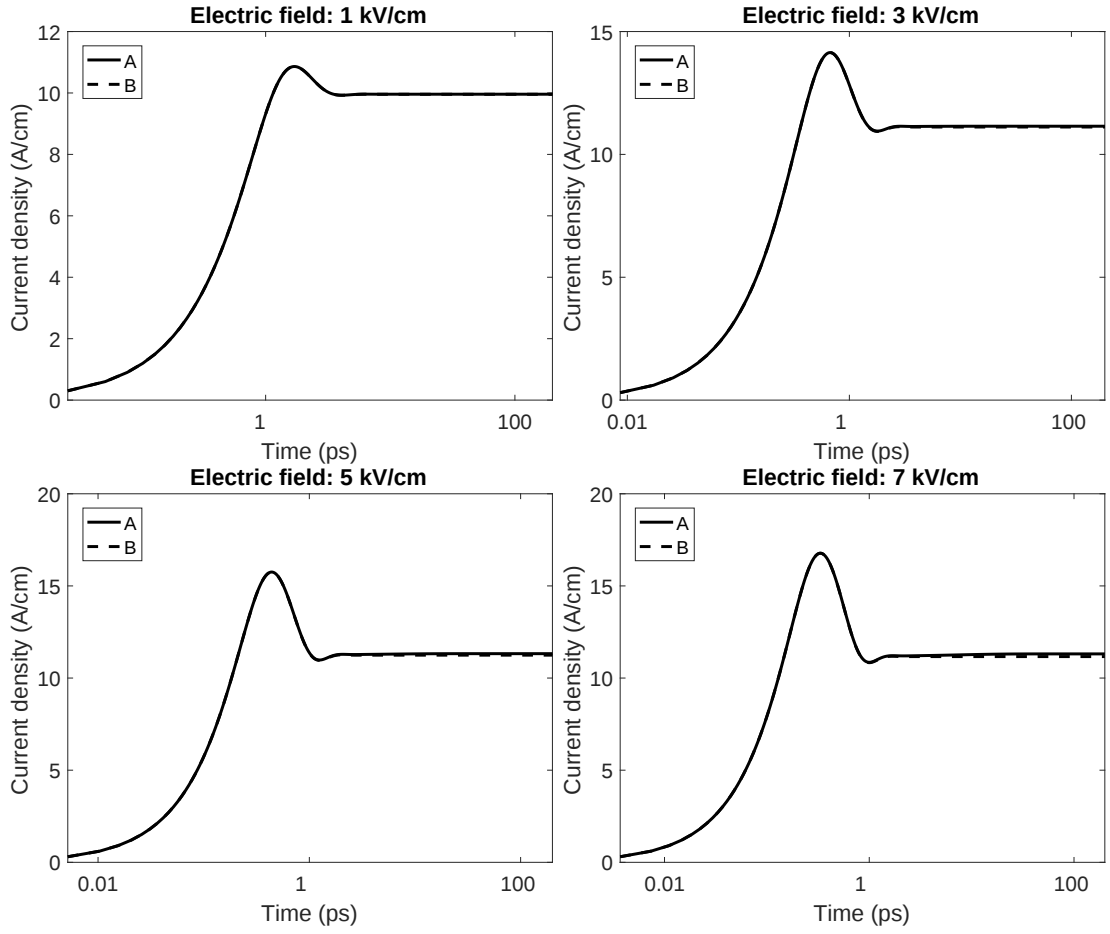


FIGURE 3.9: Total current versus time when $\varepsilon_F = 0.2$ eV under an applied electric field of 1, 3, 5, 7 kV/cm.

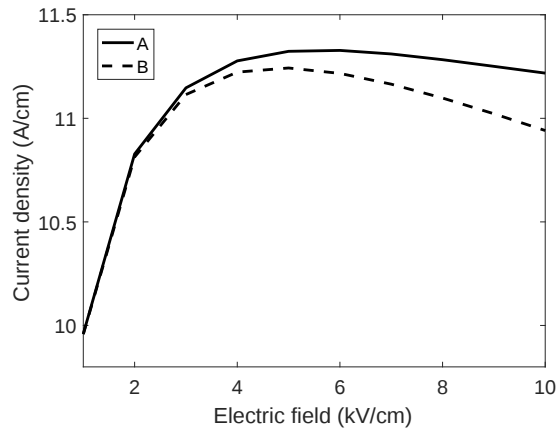


FIGURE 3.10: Steady total current versus electric field when $\varepsilon_F = 0.2$ eV.

3.3 Numerical results for graphene on h-BN

The physical setting consists of a strip of graphene which is infinitely long in the transversal direction with respect to that of the electric field, placed on an oxide substrate made of h-BN (see Fig. 3.11). As already shown in [25], the distance d is crucial for a correct prediction of the electron velocity, and therefore, in turn, of the electron mobilities. In [24] some numerical experiments have been performed in the unipolar case assuming that d is a random variable. In the present paper we assume that d is constant; in fact in [24] the results obtained with a random d are practically the same of those obtained with average values of such a parameter. This allows us to look

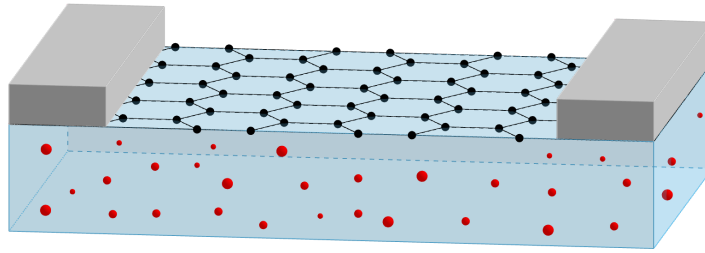


FIGURE 3.11: Schematic representation of a monolayer graphene on a h-BN substrate. In the direction parallel to the contacts the material is infinitely large. In each contact there is a constant electrostatic potential.

for solutions which are not depending on space and to avoid any effect related to the boundary conditions. As initial condition a Fermi-Dirac distribution is assumed.

Other materials have been used as substrate in the literature (see [24]), for example SiO_2 but one of the best performance is that of the h-BN on account of the lower mobility degradation. We consider several values of the Fermi energy, different applied electric fields and three choices for the parameter d , $d = 0, 0.5, 1$ nm. In Figs 3.12, 3.13, 3.14 we have compared the total steady current density $\mathbf{J}$ versus the electric field for Fermi energy $\varepsilon_F = 0, 0.05, 0.1$ eV. Note that by increasing ε_F the effect of the inclusion of the inter-band scattering reduces and the percentage of variation is less sensible to the value of d .

In the case $\varepsilon_F = 0$ eV apparently when the inter-band scatterings are taken into account the total current has a Ohmic behaviour, that is almost linear with respect to the electric field. This can be explained by the fact that the inter-band interaction promotes the formation of additional current due to the minority charge. At higher absolute values of the Fermi energy this effect vanishes, probably because the inter-band mechanism becomes weaker.

In the remaining figures the the transient solutions are shown. The steady solution is reached in about 100 picoseconds. In Fig. 3.15 the total current density is plotted

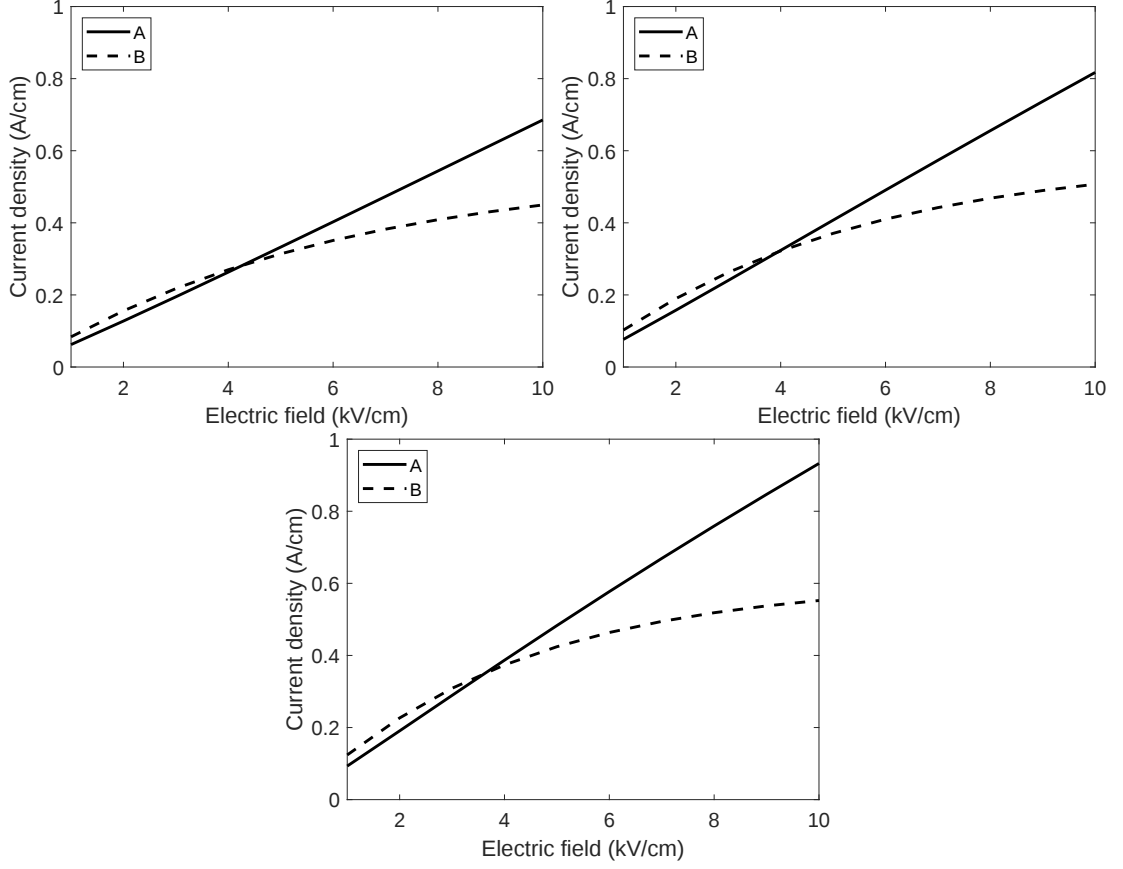


FIGURE 3.12: Steady total current versus the electric field when $\varepsilon_F = 0$ eV with (A) and without (B) inter-band scatterings in the case $d = 0$ nm (top-left), $d = 0.5$ nm (top-right) and $d = 1$ nm (bottom).

versus time for applied electric fields of 2,4,8 kV/cm. Note that for low electric fields the current obtained neglecting the inter-band transition is higher than that obtained by including it. At about 4kV/cm no difference appears while for high fields we find again a considerable variation which increases with the intensity of electric fields but now the current obtained with the inclusion of the inter-band scattering is greater and reaches the steady regime later.

In Fig. 3.16 the behaviour of the electron density versus time is reported. The behaviour of the hole density and current density is exactly the same with respect to electrons because of the symmetry in the collision operator (see [63]). Of course when the inter-band scattering is neglected the densities of both electron and holes remain constant. If $\varepsilon_F = 0.1$ eV the current has no longer a Ohmic behaviour and the characteristic curves are more similar to that of a semiconductor. In Fig. 3.17 the total current density versus time is plotted for applied electric fields of 2,4,8 kV/cm. The influence of the inter-band scattering are almost negligible for low and moderate field. An appreciable difference is detected only for electric fields higher than 8 kV/cm. In Fig. 3.18 the behaviour of the electron density and hole density versus time is reported.

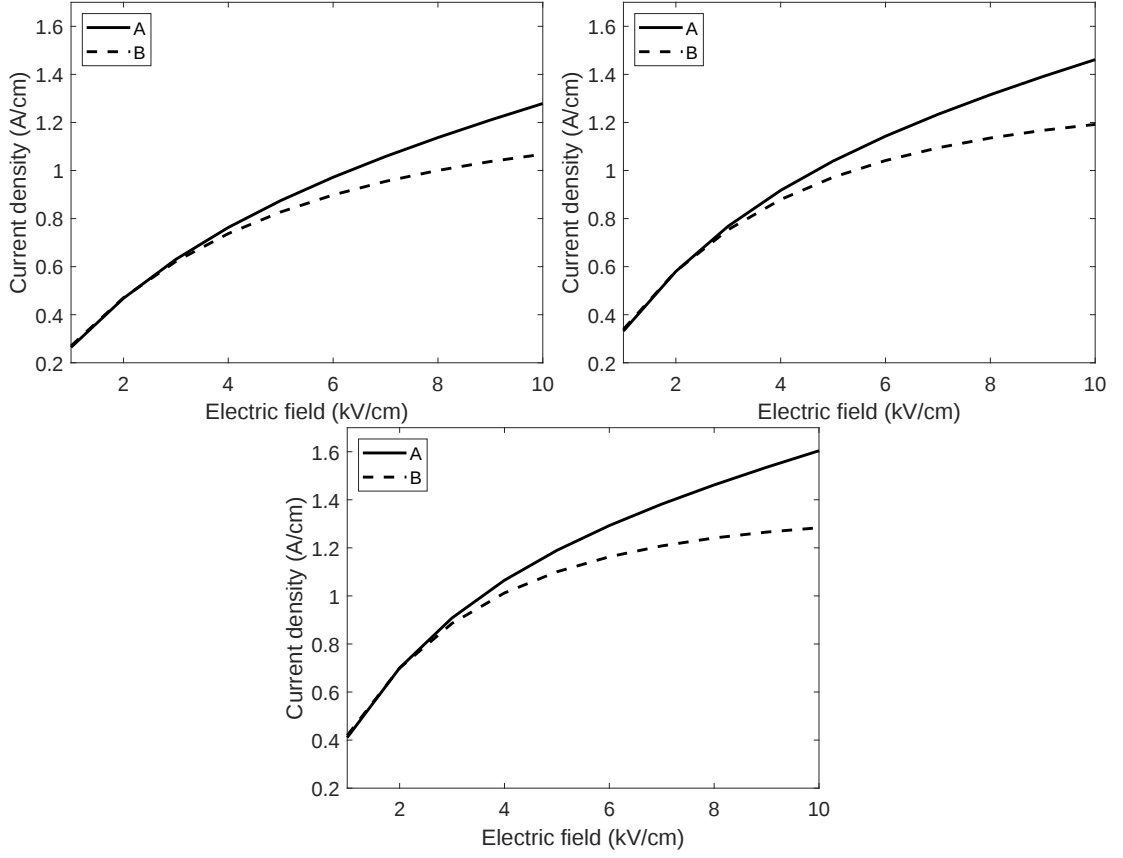


FIGURE 3.13: Steady total current versus the electric field when $\varepsilon_F = 0.05$ eV with (A) and without (B) inter-band scatterings in the case $d = 0$ nm (top-left), $d = 0.5$ nm (top-right) and $d = 1$ nm (bottom).

The behaviour of the hole density is no longer the same of that of electrons. Since the Fermi energy is positive the majority carriers are electrons. If we reverse the sign of the Fermi energy the role of electrons and holes swaps.

3.4 Conclusions

Charge transport in monolayer graphene has been simulated by a numerical deterministic approach, based on a discontinuous Galerkin (DG) method, for solving the semiclassical Boltzmann equations for electrons and holes. Both the conduction and valence bands have been included and the interband scatterings have been taken into account. The importance of the interband scatterings has been accurately evaluated for several values of the Fermi energy.

In Section 3.2 numerical simulations of a suspended monolayer graphene have been performed. It is found out that the inclusion of the interband scatterings produces, with zero Fermi energy, huge variations in the current, while, as expected, the effect of the interband scatterings becomes negligible by increasing the absolute value of the

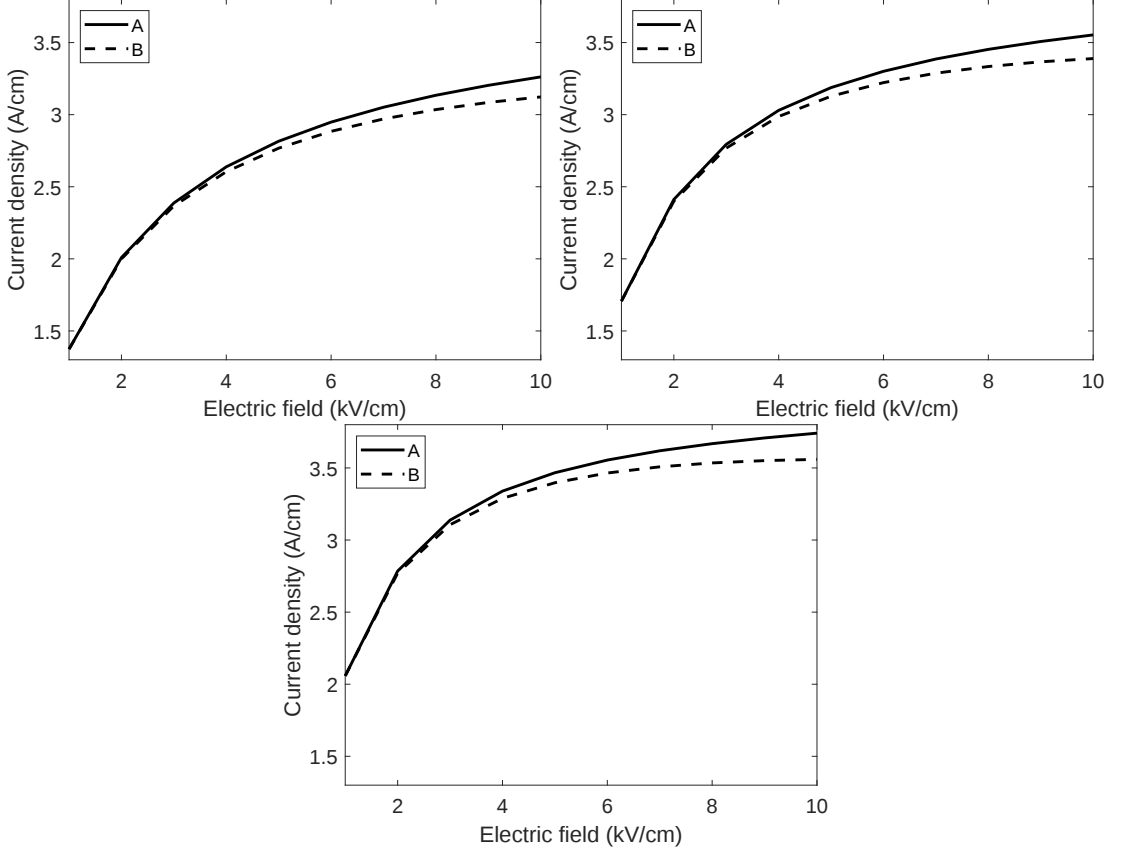


FIGURE 3.14: Steady total current versus the electric field when $\varepsilon_F = 0.1$ eV with (A) and without (B) inter-band scatterings in the case $d = 0$ nm (top-left), $d = 0.5$ nm (top-right) and $d = 1$ nm (bottom).

Fermi energy. When ε_F is greater than 0.2 eV, the interband effects can be eliminated without any significant consequence in the simulations.

In Section 3.3 an evaluation of the importance of the inter-band scattering in monolayer graphene on a h-BN substrate has been performed by adopting the same technique in the case of suspended graphene. Several values of the Fermi energy have been considered in a realistic range of applied electric fields. The inter-band interaction is relevant for values of the Fermi energy around zero eV and becomes negligible for Fermi energies in absolute value greater than 0.1 eV. The steady state is reached in about 100 picoseconds at variance of the case when the inter-band scatterings are not taken into account which requires few picoseconds to get the stationary regime. This could play a role for the on/off switching times in the application to GFETs.

As possible further improvements, the authors are investigating the inclusion of thermal effects along the results obtained for suspended monolayer graphene [26, 30] and the extraction of mobility models starting from the DG numerical results as in [62, 81].

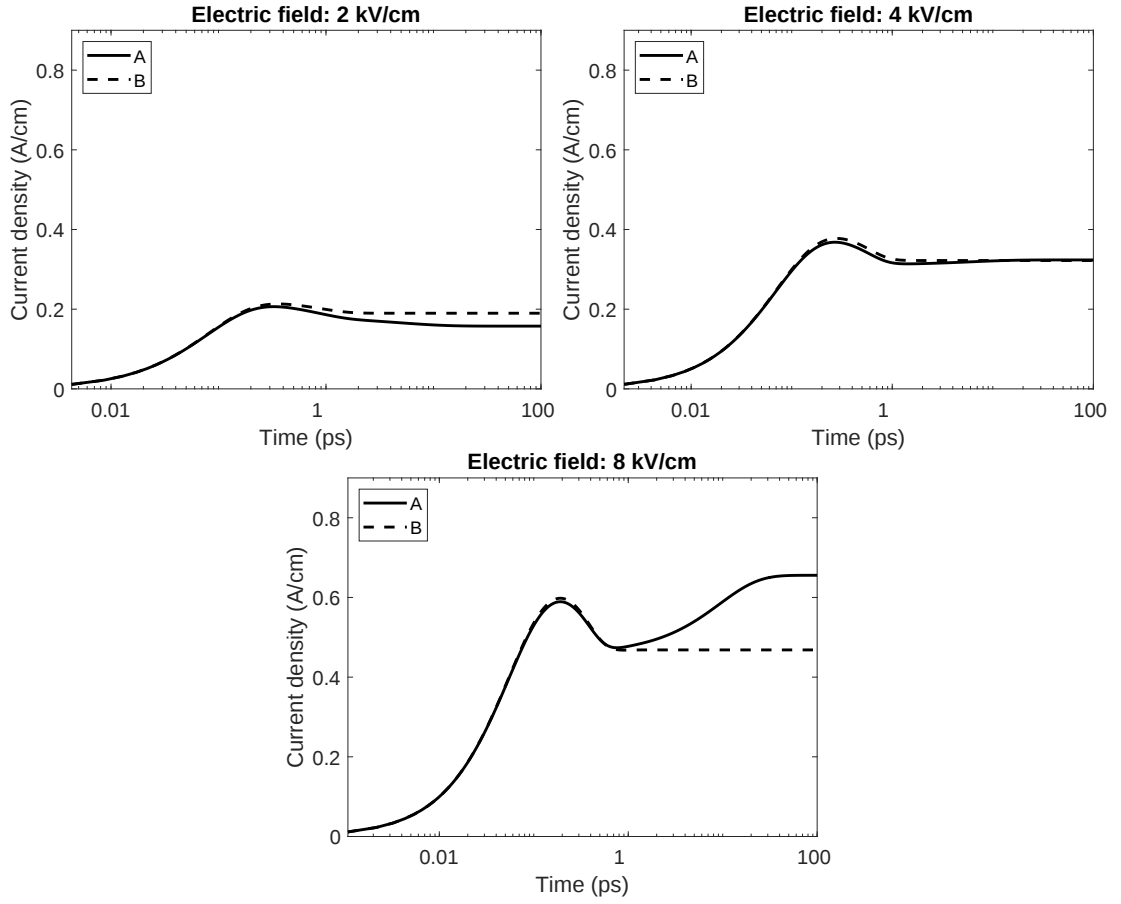


FIGURE 3.15: Total current versus time at fixed values of electric field in the case $\varepsilon_F = 0$ eV with (A) and without (B) inter-band scatterings in the case $d = 0.5$ nm.

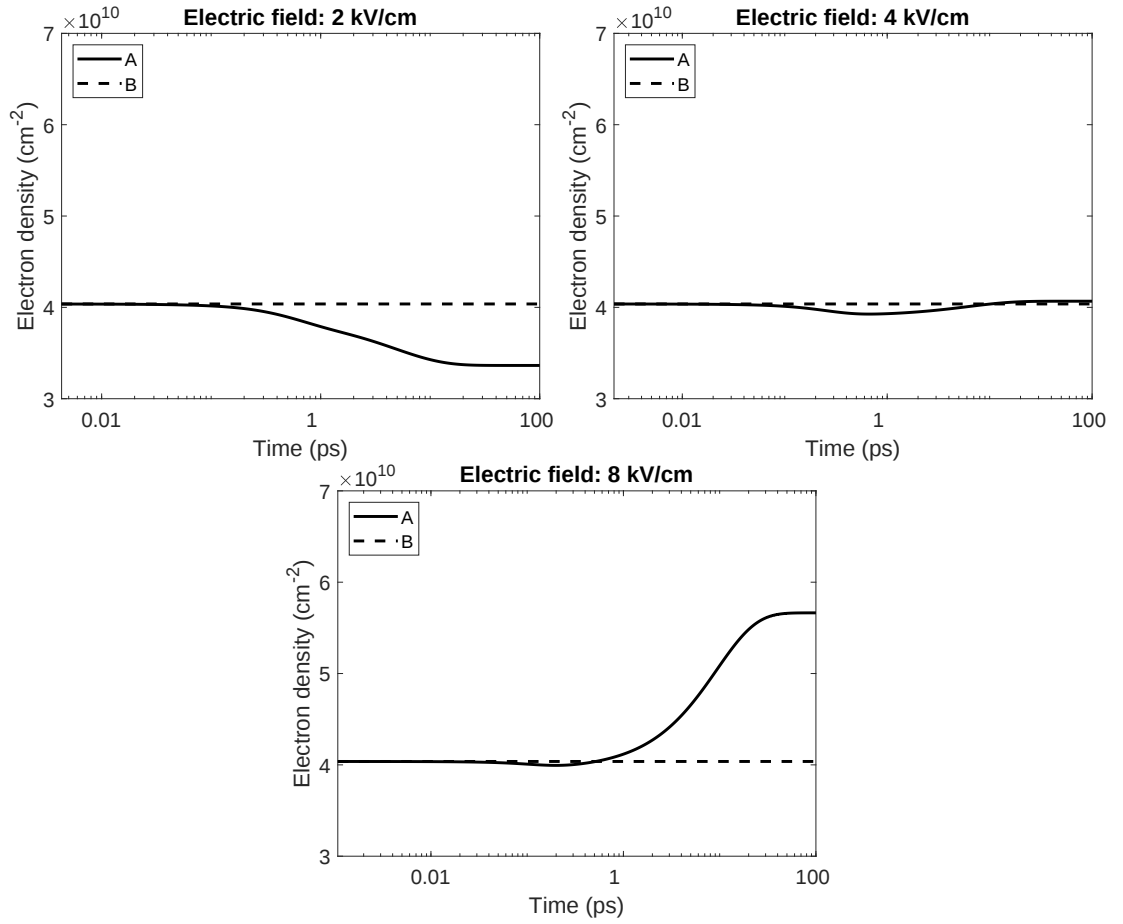


FIGURE 3.16: The electron density versus time at fixed values of electric field in the case $\varepsilon_F = 0$ eV with (A) and without (B) inter-band scatterings in the case $d = 0.5$ nm. The solutions for holes are exactly the same.

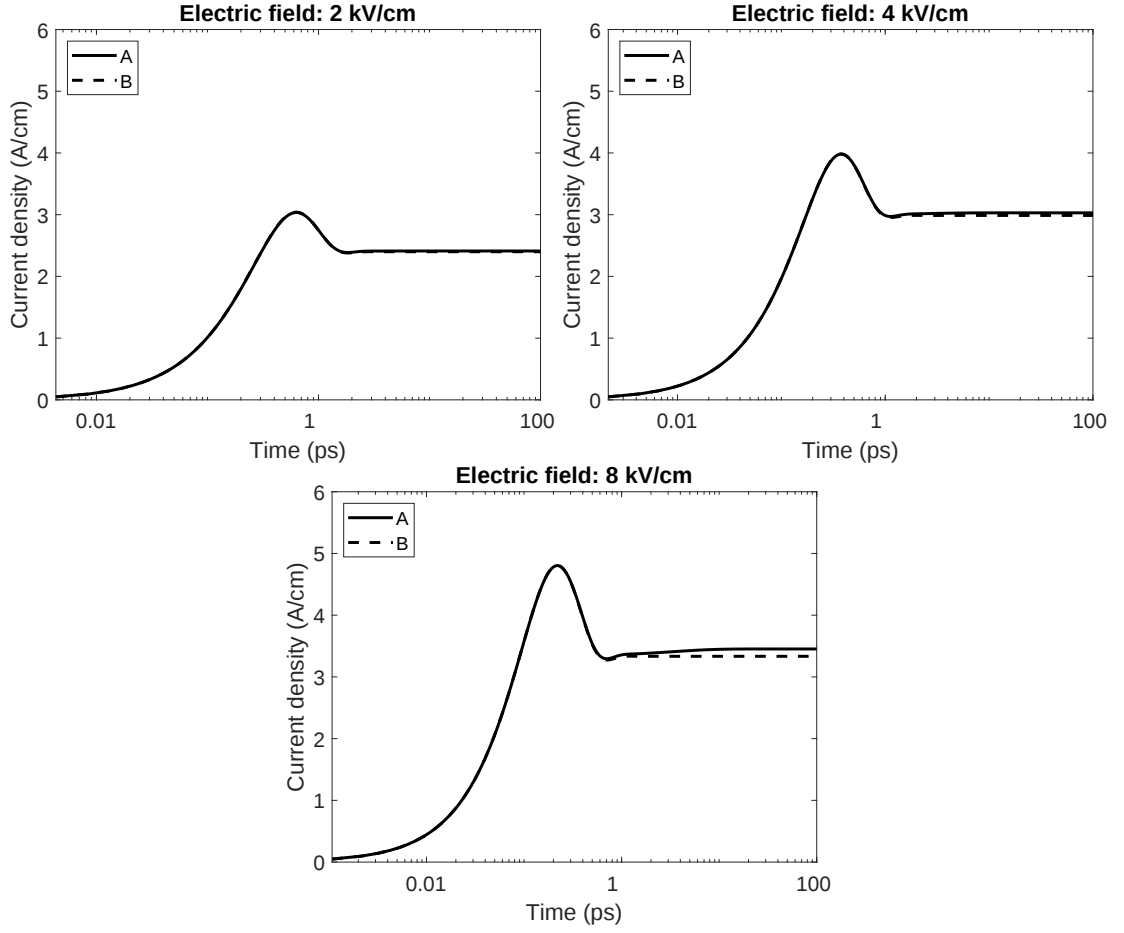


FIGURE 3.17: Total current versus time at fixed values of electric field in the case $\varepsilon_F = 0.1$ eV with (A) and without (B) inter-band scatterings in the case $d = 0.5$ nm.

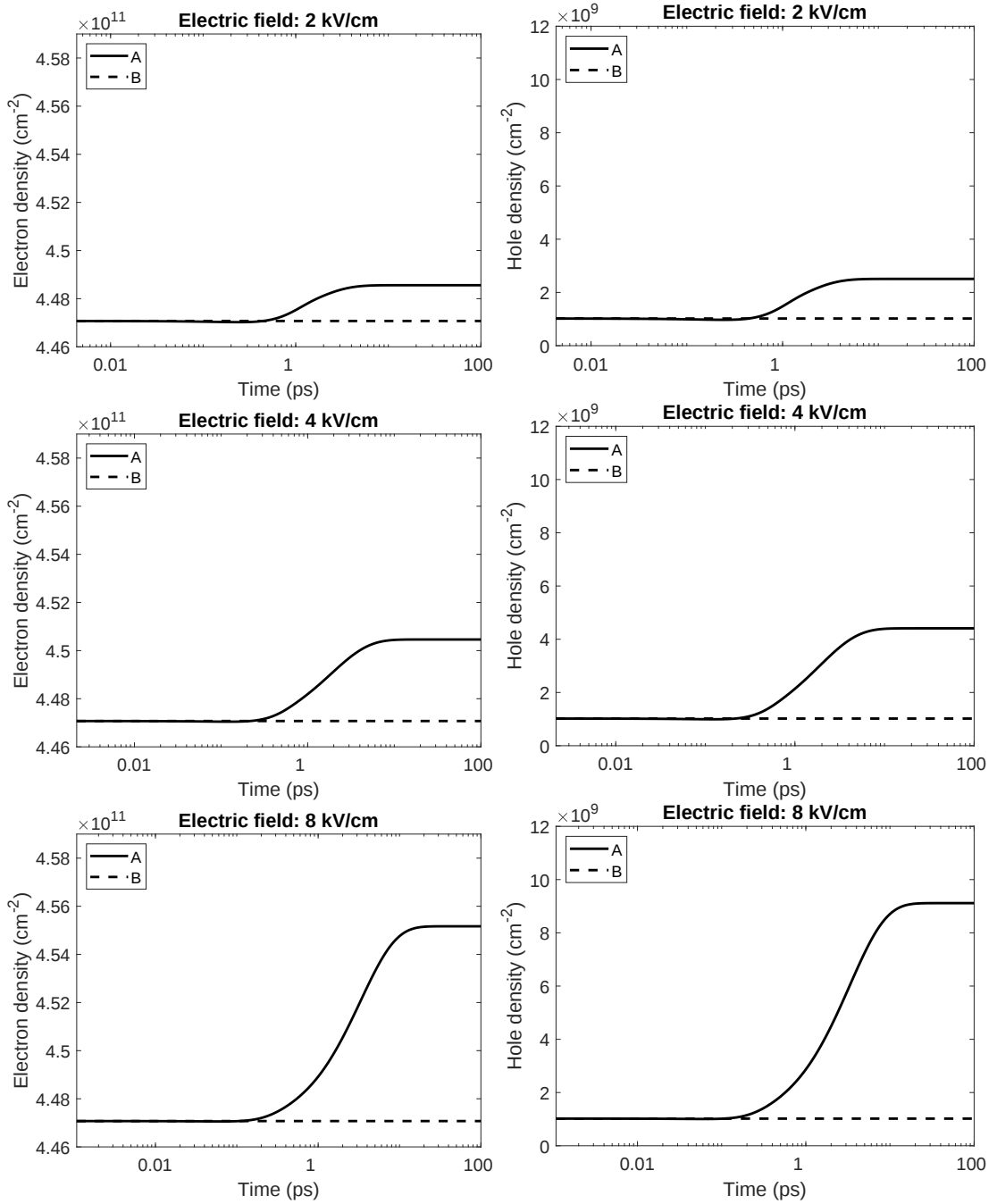


FIGURE 3.18: The electron density (left) and hole density (right) versus time at fixed values of electric field in the case $\varepsilon_F = 0.1$ eV with (A) and without (B) inter-band scatterings in the case $d = 0.5$ nm. The solutions for holes are exactly the same.

Chapter 4

Mobility models and applications to GFETs

Charge transport in graphene is crucial for the design of a new generation of nanoscale electron devices. As already discussed in Chapter 3, a reasonable model is represented by the semiclassical Boltzmann equations for electrons in the valence and conduction bands. As shown in [89], the discontinuous Galerkin methods are a viable way to tackle the problem of the numerical integration of these equations, even if efficient DSMC with a proper inclusion of the Pauli principle have been also devised. One of the advantages of the solutions obtained with deterministic approach is of course the absence of statistical noise. This fact is crucial for an accurate estimation of the low field mobility as proved in the case of a unipolar charge transport in a suspended graphene sheet under a constant electric field [62].

The mobility expressions are essential for the drift-diffusion equations which constitute the most adopted models for charge transport in CAD. In Section 1 we present an improvement with respect to the analysis of [62]. New models of mobility are obtained and, in particular, relevant improvements of the low field mobility are achieved [81]. If graphene is placed on a substrate a crucial parameter is the distance between the graphene layer and the impurities due to the substrate. Measurements demonstrate that this distance is of the order of a few angstroms. The first choice can be to set this parameter constant while another choice consists to model the impurity distribution with a random variable and include it in a DSMC simulation. In Section 2 we show numerical results of this second choice, presented in [24]. However the main conclusion is that the expected value of the distribution is the dominant parameter and this suggests that the constant choice is accurate enough. In Section 3 a mobility model which takes into account the presence of a double layer (top and bottom) of oxide substrate is outlined. The last part of this chapter is devoted to the GFET simulations. A GFET is a field effect transistor where the active area is made of a monolayer graphene. In Section 4 we present numerical simulation of a GFET first exploring the mobility model proposed in [33] and next adopting the mobility model based on the

Boltzmann equation [79].

We remark that the results of this chapter are original and presented in Ref.s [81, 24, 79, 82].

4.1 The mobility model in the case of suspended monolayer graphene

The mobility expressions are essential for the drift-diffusion equations which constitute the most adopted models for charge transport in CAD. Here the analysis in [62] is improved in two ways: by including the charge transport both in the valence and conduction bands, and by taking into account the presence of an oxide as substrate for the graphene sheet.

In this section a new mobility model is presented in the case of suspended monolayer graphene and comparisons with other models already existing in the literature are performed. In Section 4.3 a further extension is presented for graphene on a substrate made of silicon dioxide.

4.1.1 Model and method description

For applications in electronic device modeling, in order to reduce the computational effort, macroscopical models are mostly adopted. The simplest and most popular ones are the drift-diffusion (DD) models. They have been already described in Section 1.4, where was remarked that the mobility models are crucial for the correct determination of the current.

The mobilities are definite through the relations (in the one dimensional case)

$$v_n = \mu_n(E, n)E, \quad v_h = \mu_p(E, p)E, \quad (4.1)$$

where E , v_n and v_p are the significant components of the the electric field, the average electron velocity and the average hole velocity. The velocities are related to the currents as follows

$$v_n = J_n/n, \quad v_h = J_p/p.$$

First we analyze the low field mobility μ_0 , that is defined as

$$\mu_0(n) = \lim_{E \rightarrow 0} \mu_n(E, n). \quad (4.2)$$

In principle the low field mobilities of electron and holes are different. In suspended graphene they take the same values.

The main concern regarding the low field mobility is that its determination from experimental data is rather cumbersome on account of the intrinsic statistical noise. A similar issue arises if the results obtained by DSMC are employed. The use of the results given by the DG approach avoids such difficulties because reduces (practically avoids) the effects of the statistical noise.

For the determination of the mobility curves it is enough to consider homogeneous solutions of the semiclassical Boltzmann equation numerically solved by means of the DG method. In this section we examine the case of a suspended single sheet of graphene, as reported in Figure 1.5. We suppose that the contacts are deeply infinite and the potential is constant in each of them. Therefore, the electric field is constant and transversal with respect to the contact. Thus the system can be solved in the interval $[0, L]$ with Dirichlet boundary conditions

$$n|_{x=0} = n_0, \quad n|_{x=L} = n_L, \quad p|_{x=0} = p_0, \quad p|_{x=L} = p_L.$$

The solution does not depend on space.

For several values of n corresponding to a Fermi level between 0 eV and 0.4 eV, the low field mobility is extrapolated, by a linear regression model, computing the mobility at different low values of electric field, between $0.0005 \text{ V}/\mu\text{m}$ and $0.0025 \text{ V}/\mu\text{m}$, by using the values of the currents obtained by a direct solution of the Boltzmann equation with the DG method outlined in previous chapters. One observes (see Figure 4.1) that the low field mobility behaviour versus the density (or equivalently the Fermi energy) is similar to the log-normal distribution and therefore we assume the following expression

$$\mu_0(n) = \tilde{\mu}_0 \frac{\exp\left(-\frac{(\log(n/n_{ref})-m)^2}{2\sigma^2}\right)}{\sqrt{2\pi\sigma n/n_{ref}}}, \quad (4.3)$$

where $\tilde{\mu}_0$, n_{ref} , m and σ are fitting parameters. The behaviour is the same for holes on account of the symmetry between the hole and electron distributions.

We have estimated the parameters by means of the least squares method. The obtained values are reported in Table 4.1.

$\tilde{\mu}_0$	n_{ref}	m	σ
$217.07 \mu\text{m}^2/\text{V ps}$	$8951.4 \mu\text{m}^{-2}$	-0.0027671	1.3423

TABLE 4.1: Low field mobility parameters.

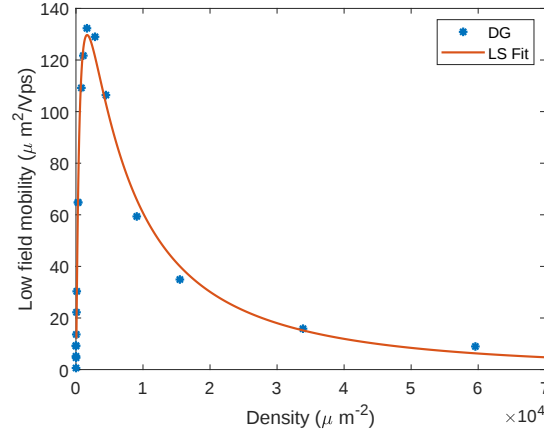


FIGURE 4.1: Comparison between the low field mobility simulated with the DG method and the fitted one.

As second step, we include the electric field dependence by proposing the same model of Ref. [62]

$$\mu(E, n) = \frac{\mu_0(n) + \frac{v_F}{E} \left(\frac{E}{E_{ref}} \right)^{\beta_1}}{1 + \left(\frac{E}{E_{ref}} \right)^{\beta_2} + \gamma \left(\frac{E}{E_{ref}} \right)^{\beta_3}}, \quad (4.4)$$

where E_{ref} , β_1 , β_2 , β_3 and γ are fitting parameters. In this case we evaluated the mobility by means of the DG results of the transport equations at different densities, corresponding to the Fermi levels of 0.2 eV, 0.3 eV, 0.4 eV, and for a range of electric fields between 0.025 V/ μm and 10 V/ μm . The obtained parameters are reported in Table 4.2. A comparison between fitted and simulated values of mobility models and

E_{ref}	β_1	β_2	β_3	γ
0.0421 V/ μm	1.2898	1.4050	0.9627	5.0918

TABLE 4.2: Mobility model parameters.

corresponding current densities are plotted in Figure 4.2

4.1.2 Comparison with other mobility models

There are available in the literature several expressions of the mobilities. Most of them are based on heuristic considerations or experimental data. A widely used model is that of Dorgan et al. [33]

$$\mu(x) = \frac{v}{[1 + (vE/v_{sat})\gamma]^{1/\gamma}},$$

where v_{sat} is the saturation velocity, $\gamma \approx 2$ and

$$v(x) = \frac{\mu_0}{(1 + n/n_{ref})^\alpha},$$

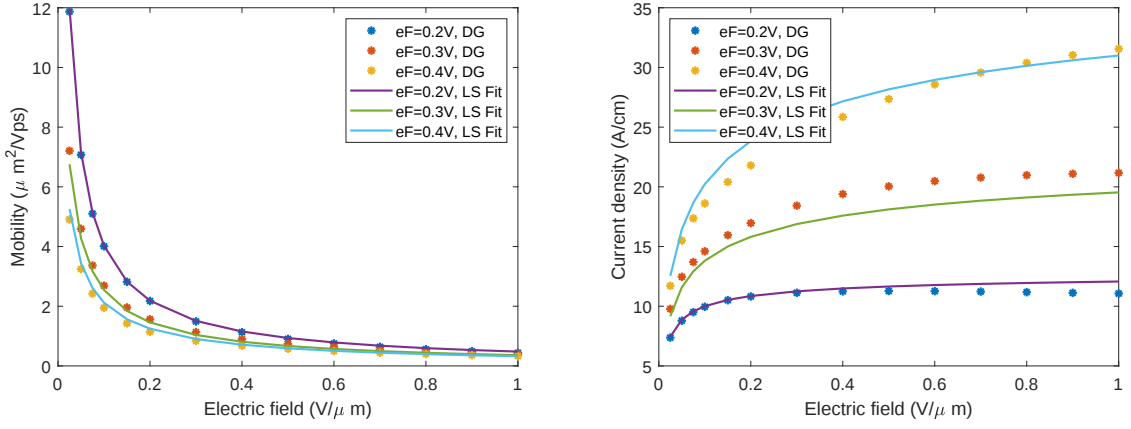


FIGURE 4.2: On the left comparison between the mobility simulated with the DG method and the fitted one. On the right the comparison of the simulated and fitted current densities for several values of the Fermi energy.

with μ_0 the low field mobility, $n_{ref} = 1.1 \times 10^5 \mu\text{m}^{-2}$ and $\alpha = 2.2$.

In [33] the value $\mu_0 = 0.4650 \mu\text{m}^2/\text{V ps}$ is taken while the saturation velocity is evaluated as

$$v_{sat} = \frac{2}{\pi} \frac{\omega_{OP}}{\sqrt{\pi n}} \sqrt{1 - \frac{\omega_{OP}^2}{4\pi n v_F^2} \frac{1}{N_{OP} + 1}} \quad (4.5)$$

where $\hbar\omega_{OP}$ is the energy of optical phonons, that here takes the value of 160 meV, and

$$N_{OP} = \frac{1}{\exp\left(\frac{\hbar\omega_{OP}}{k_B T}\right) - 1} \quad (4.6)$$

is the phonon occupation number. The previous expressions, written for the electron density n , are still valid for the hole density p . Here for the saturation velocity the values reported in Table 4.3 have been adopted.

eF	v_{sat}
0.2 eV	0.5841 $\mu\text{m}/\text{ps}$
0.3 eV	0.4393 $\mu\text{m}/\text{ps}$
0.4 eV	0.3426 $\mu\text{m}/\text{ps}$

TABLE 4.3: Adopted saturation velocity values.

In Ref. [62] the authors used the model given by the equation (4.4) but with a different expression of the low field mobility

$$\mu_0 = \mu_0(n) = \frac{\tilde{\mu}}{1 + (n/n_{ref})^\alpha} \quad (4.7)$$

(a similar expression can be introduced also for holes) with $n_{ref} = 0.5 \times 10^4 \mu\text{m}^{-2}$,

$\alpha = 1.2916$ and $\tilde{\mu} = 2\mu_0(n_{ref}) = 373.4306 \mu\text{m}^2/\text{V ps}$. The reader is referred to [62] for the specific values of the parameters.

In Figure 4.3 we have compared the different mobility curves among them and with the results of the direct solution of the transport equations in the case of a Fermi energy 0.2 eV (top left). In the figure we have also included a modified Dorgan model (MDM) where the low field mobility is taken as that given by relation (4.3).

The model of Dorgan et al. underestimates the mobility, in particular for low fields. MDM and the model in [62] are in good agreement between them but there is a considerable discrepancy with the results given by the Boltzmann equation. Apparently the inclusion of the interband scattering, neglected in [62], has a relevant role for a correct determination of the low field mobility. At high fields all the mobility curves become closer.

In Figure 4.3 (top right and bottom) Fermi energies of 0.3 eV and 0.4 eV are considered. In these plots the original model of Dorgan et al. is not reported because of the high discrepancy. In the case of a Fermi energy of 0.3 eV the model in [62] is more accurate than MDM for low fields. In the case of a Fermi energy of 0.4 eV the model in [62] is more accurate than MDM for low fields but less accurate for high fields.

4.1.3 The mobility model in the case of graphene on substrate

In order to include the presence of a substrate as depicted in Figure 4.4, a further generalization of the mobility model is required. In this situation usually one observes a degradation of the current due to the additional scatterings of the charges in the graphene with the phonons and impurities in the substrate. We have considered the case of graphene on SiO_2 (silicon dioxide) and again used a DG method for solving the transport equations (the interested reader is referred to [25, 24] for details).

A crucial parameter, entering the expression of the collision term, is the average distance d between the graphene and the impurities. The value of d is considered to lie in the range between 0 and 1 nm. We have obtained the mobility curves for some values of d by using again relations (4.3) and (4.4).

The fitted parameters are reported in Table 4.4. The obtained mobilities and current densities are shown in Figures 4.5, 4.6 and 4.7 considering $d = 0, 0.5, 1$ nm and several values of the Fermi energy.

d	E_{ref}	β_1	β_1	β_1	γ
0 nm	0.4879 V/ μm	2.0736	0.8672	1.6147	4.9884
0.5 nm	0.3875 V/ μm	1.9923	2.3816	1.2336	4.8663
1 nm	0.3626 V/ μm	1.8753	2.0545	1.1854	5.6979

TABLE 4.4: Mobility model parameters on SiO_2 .

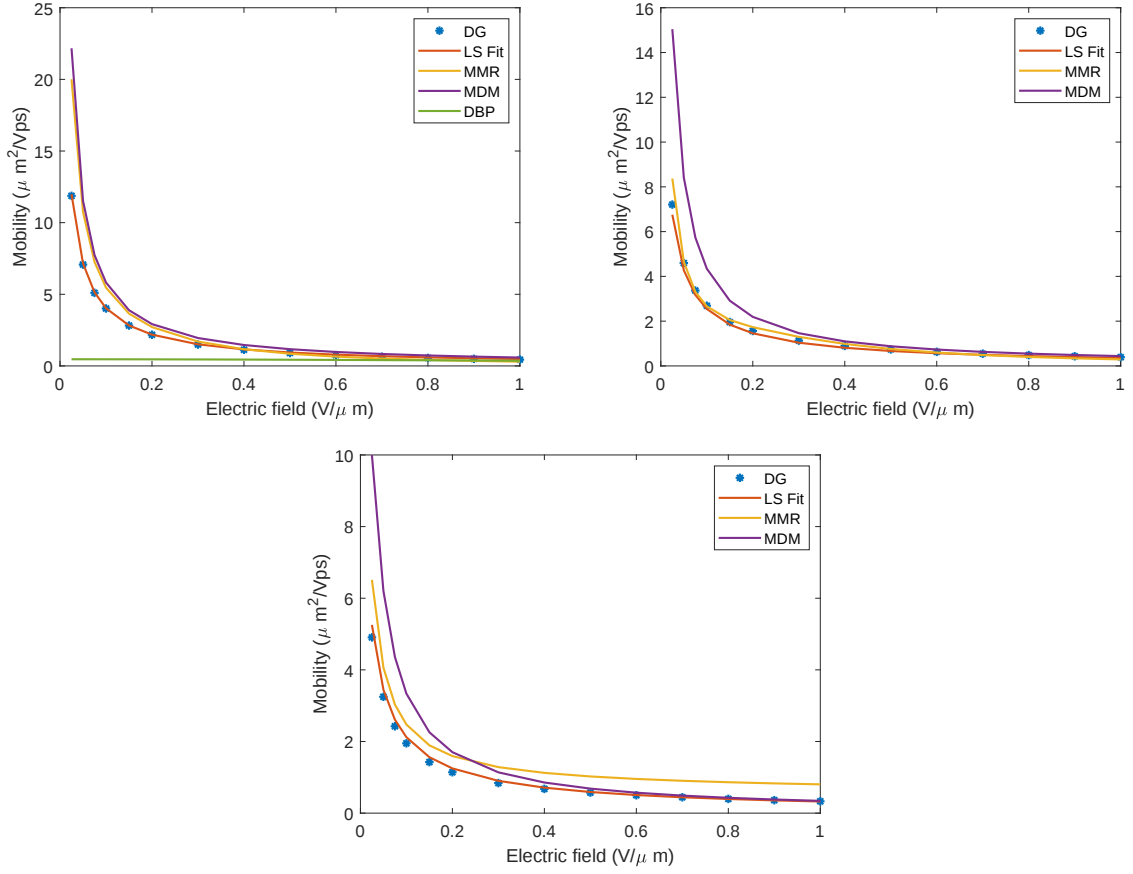


FIGURE 4.3: Comparison among the mobility models of Ref. [62] (MMR) and Ref. [33] (MDM) and the fitted one with respect to the DG simulations at a Fermi level of 0.2 eV (top left), 0.3 eV (top right) and 0.4 eV (bottom). At the Fermi level of 0.2 eV it is also shown the original model of Ref. [33] (DBP).

As expected we have a degradation of the mobility which reduces by increasing d . The latter effect is easily explained because there is a reduction of the scattering rate with impurities as the distance increases between the graphene sheet and the impurities in the oxide.

4.2 DSMC simulations of graphene on substrate

In this section we present the simulation of charge transport in a monolayer graphene on different substrates. This requires the inclusion of the scatterings of charge carriers with impurities and phonons of the substrate, besides the interaction mechanisms already present in the graphene layer. As mathematical model, the semiclassical Boltzmann equation is assumed and the results are based on Direct Simulation Monte Carlo

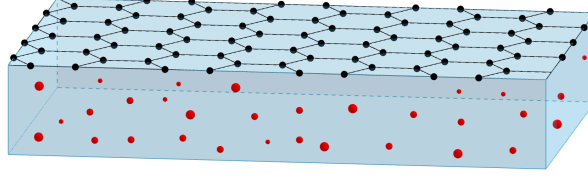


FIGURE 4.4: Schematic representation of a graphene sheet on a substrate. The dots stand for the impurities in the oxide.

d	μ_0 ($eF = 0.2$ eV)	μ_0 ($eF = 0.3$ eV)	μ_0 ($eF = 0.4$ eV)
0 nm	$2.867 \mu\text{m}^2/\text{V ps}$	$1.252 \mu\text{m}^2/\text{V ps}$	$0.676 \mu\text{m}^2/\text{V ps}$
0.5 nm	$4.106 \mu\text{m}^2/\text{V ps}$	$2.123 \mu\text{m}^2/\text{V ps}$	$1.353 \mu\text{m}^2/\text{V ps}$
1 nm	$5.704 \mu\text{m}^2/\text{V ps}$	$3.345 \mu\text{m}^2/\text{V ps}$	$2.366 \mu\text{m}^2/\text{V ps}$

TABLE 4.5: Low field mobility on SiO_2 .

(DSMC) method. A crucial point is the correct inclusion of the Pauli Exclusion Principle (PEP). Most simulations use the approach proposed in [60] which, however, allows an occupation number greater than one with an evident violation of PEP. Here the Monte Carlo scheme devised in [89] is employed. It predicts occupation numbers consistent with PEP and therefore is physically more accurate.

Two different substrates are investigated: SiO_2 and hexagonal boron nitride (h-BN). We adopt the model for charge-impurities scattering described in Ref. [43]. In such a model a crucial parameter is the distance d between the graphene layer and the impurities of the substrate. Usually d is considered constant [25]. Here we assume that d is a random variable in order to take into account the roughness of the substrate and the randomness of the location of the impurities.

The results confirm that h-BN is one of the most promising substrate also for the high-field mobility on account of the reduced degradation of the velocity due to the remote impurities. This is in agreement with results shown in [42] where only the low-field mobility has been investigated.

We remark that the results presented in this section are included in [24].

4.2.1 Numerical results

In this section the semiclassical Boltzmann equation with the inclusion of electron-substrate interaction is solved for high values of the Fermi level that allow us to neglect the contribution of electrons in the valence band. The adopted DSMC procedure has been already described in Section 2.2. The simulations are performed at several values of the electric field and Fermi energy.

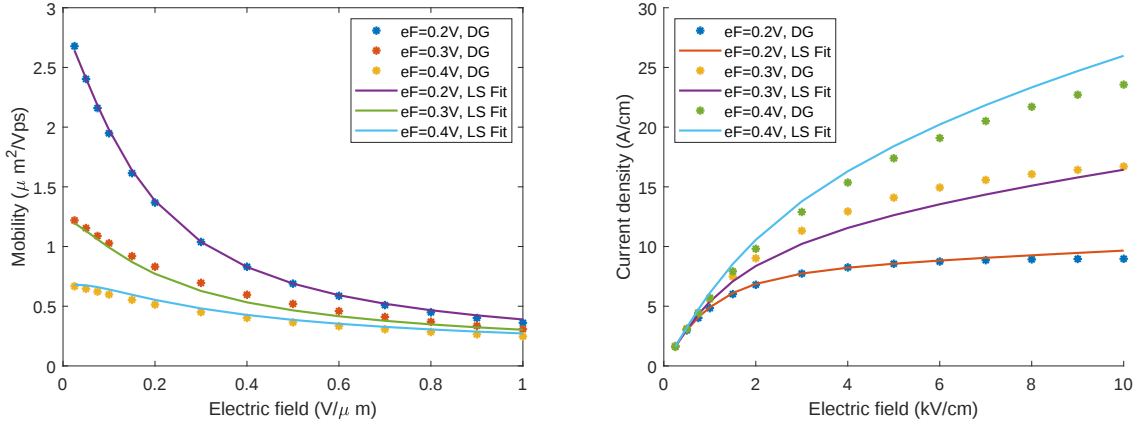


FIGURE 4.5: On the left comparison between the simulated by DG and the fitted mobility models in the case of graphene on SiO_2 with a distance between the graphene sheet and impurities of $d = 0$ nm. On the right the same for the densities.

In order to validate the simulation approach, we numerically solve, in the case of constant d , the Boltzmann equation by using a DG method (see [25] for the details), obtaining an excellent agreement.

The parameter d should be of the order of few angstroms. In the literature a range from 0 to 1 nm is considered. At variance with [25], d is considered a random variable. Therefore, in the simulation whenever a scattering with impurities occurs, d is generated according to the chosen distribution. We compare DSMC results, considering d both constant and random, with the numerical solutions of the Boltzmann equation obtained by using DG method with a constant d only.

Conservation of the number of electrons implies that the charge density ρ , given by

$$\rho = \frac{2}{(2\pi)^2} \int_{\mathbb{R}^2} f(t, \mathbf{k}) d\mathbf{k}, \quad (4.8)$$

is constant in time.

We choose a reference frame such that only the x -component of the electric field is different from 0; therefore only the x -component of the mean velocity is relevant. 10^5 particles have been used in the DSMC method.

In Figs. 4.8-4.10, we show the numerical results of the average velocity $\mathbf{v}$ defined as

$$\mathbf{v}(t) = \frac{2}{(2\pi)^2 \rho} \int_{\mathbb{R}^2} f(t, \mathbf{k}) \frac{1}{\hbar} \nabla_{\mathbf{k}} \varepsilon(\mathbf{k}) d\mathbf{k}, \quad (4.9)$$

and is related to the mobility $\mu(\mathbf{E})$ as follows

$$\mathbf{v} = \mu(\mathbf{E})\mathbf{E}.$$

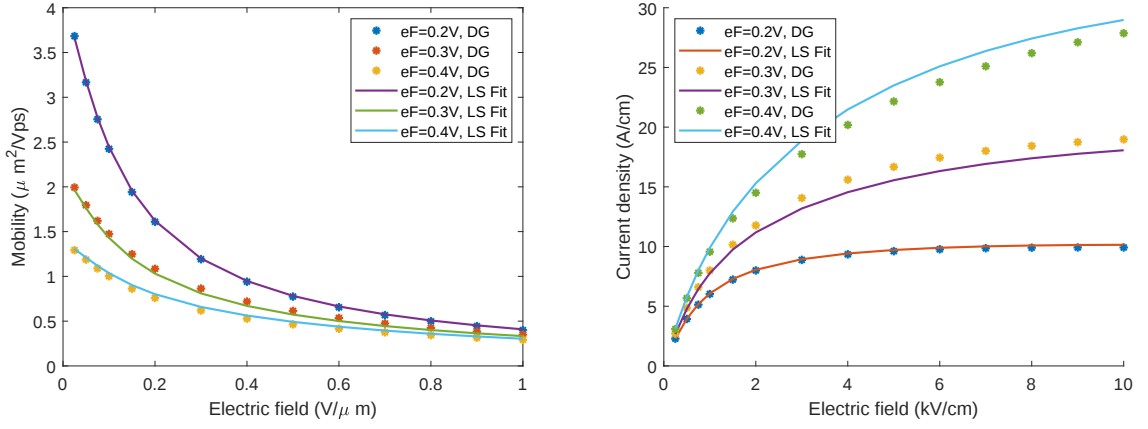


FIGURE 4.6: On the left comparison between the simulated by DG and the fitted mobility models in the case of graphene on SiO_2 with a distance between the graphene sheet and impurities of $d = 0.5 \text{ nm}$. On the right the same for the densities.

The current $\mathbf{J}$ is given by

$$\mathbf{J} = -e\rho\mathbf{v}.$$

From the analysis of the average velocity, it is possible to estimate the effect of the impurities on the mobility. It is expected that the scattering with the remote impurities leads to a degradation of the mobility depending on the specific material.

First, we have assessed the general performance of the different materials by a comparison of the average velocity for three different constant values of d .

We observe that the values of the average velocity and energy become lower by reducing the distance d from the impurities in the oxide, confirming the degradation of the mobility due to the substrate as a direct consequence of the additional scatterings with the remote impurities. For the highest value of d , which is very close to the pristine case, both SiO_2 and h-BN produce of course the same effect, with a comparable electron velocity. For the intermediate value of d , h-BN performs better than SiO_2 and this behavior is even more evident for $d = 1 \text{ nm}$. Therefore, h-BN gives a better high-field mobility, in qualitative agreement with the low field analysis in [42].

The previous results, however, do not take into account the intrinsic noise in the location of the impurities. In order to assess its effect on the high-field mobility, we have performed some simulations with a random d generated, in each scattering involving impurities, according to a prescribed probability distribution (see Fig. 4.10). First we have considered a uniform distribution in the interval $[0, 1]$ (in nm). The results are similar to those of the case with constant $d = 0.5 \text{ nm}$ and this can be explained by observing that 0.5 is the expectation value. Afterwards, we have considered a $\Gamma(\alpha, \lambda)$

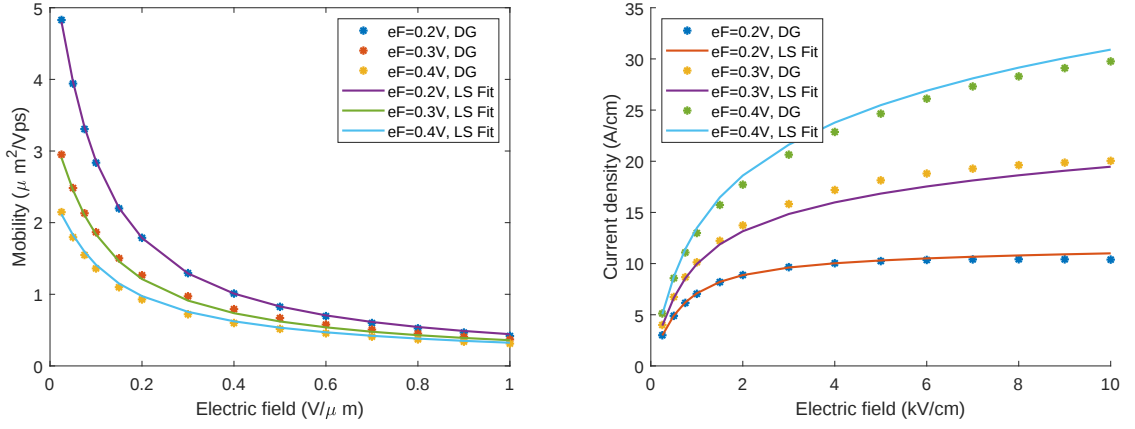


FIGURE 4.7: On the left comparison between the simulated by DG and the fitted mobility models in the case of graphene on SiO_2 with a distance between the graphene sheet and impurities of $d = 1 \text{ nm}$. On the right the same for the densities.

distribution

$$f(x) = \begin{cases} \frac{1}{\lambda \Gamma(\alpha)} x^{\alpha-1} e^{-x/\lambda} & x > 0 \\ 0 & x \leq 0 \end{cases}$$

where $\Gamma(\alpha)$ is the Euler gamma function. We have used the values $\lambda = 0.5$ and $\alpha = 2, 3, 4$ (see Fig. 4.11) and rescaled d by a factor 0.2 in order to have values less than 1 with very high probability, as confirmed by the simulation.

In order to validate our findings, the results obtained by using the DG method in [25] but with a value of d set equal to the mean values of the considered distribution (the mean value of $\Gamma(\alpha, \lambda)$ is $\alpha\lambda$) rescaled by the factor 0.2. The agreement is still excellent.

We would like to remark by observing that both the materials seem only slightly influenced by the stochastic effect related to the randomness of the impurity positions.

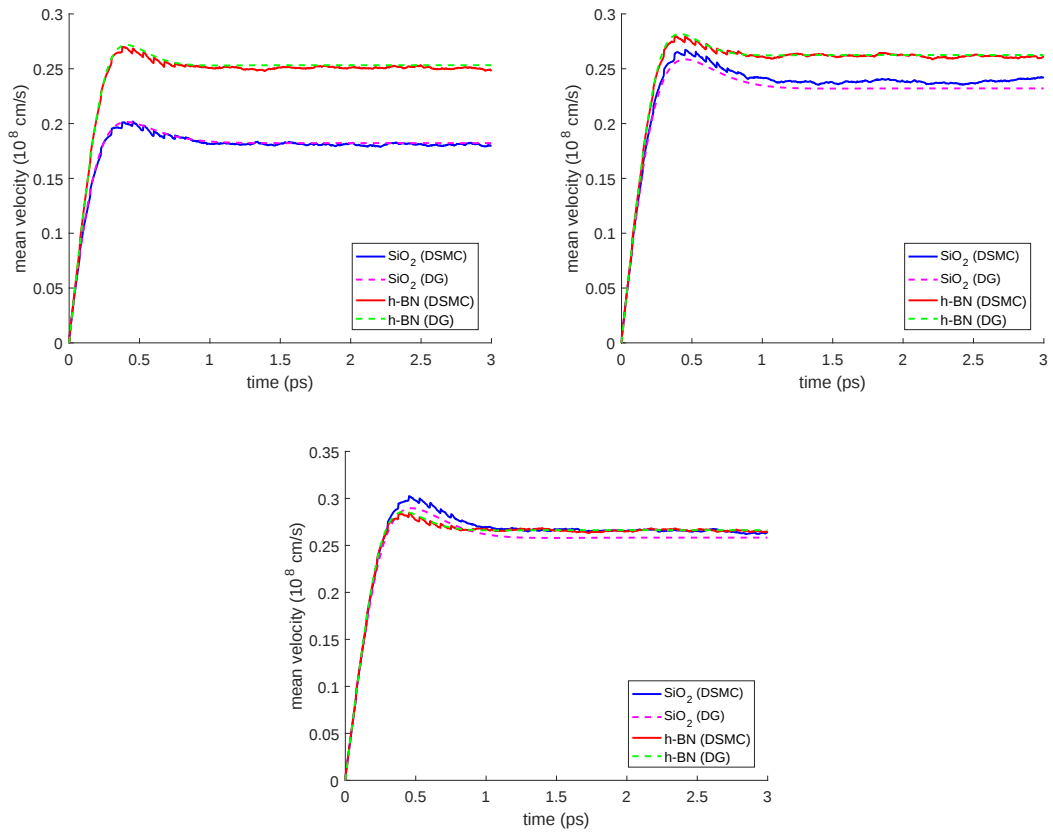


FIGURE 4.8: Comparison of the average velocity versus time for d equal to 0 nm (top-left), 0.5 nm (top-right), 1 nm (bottom) in the case of an applied electric field of 5 kV/cm and Fermi energy $\varepsilon_F = 0.4$ eV. Both the results obtained by using the DSMC and the DG method are reported.

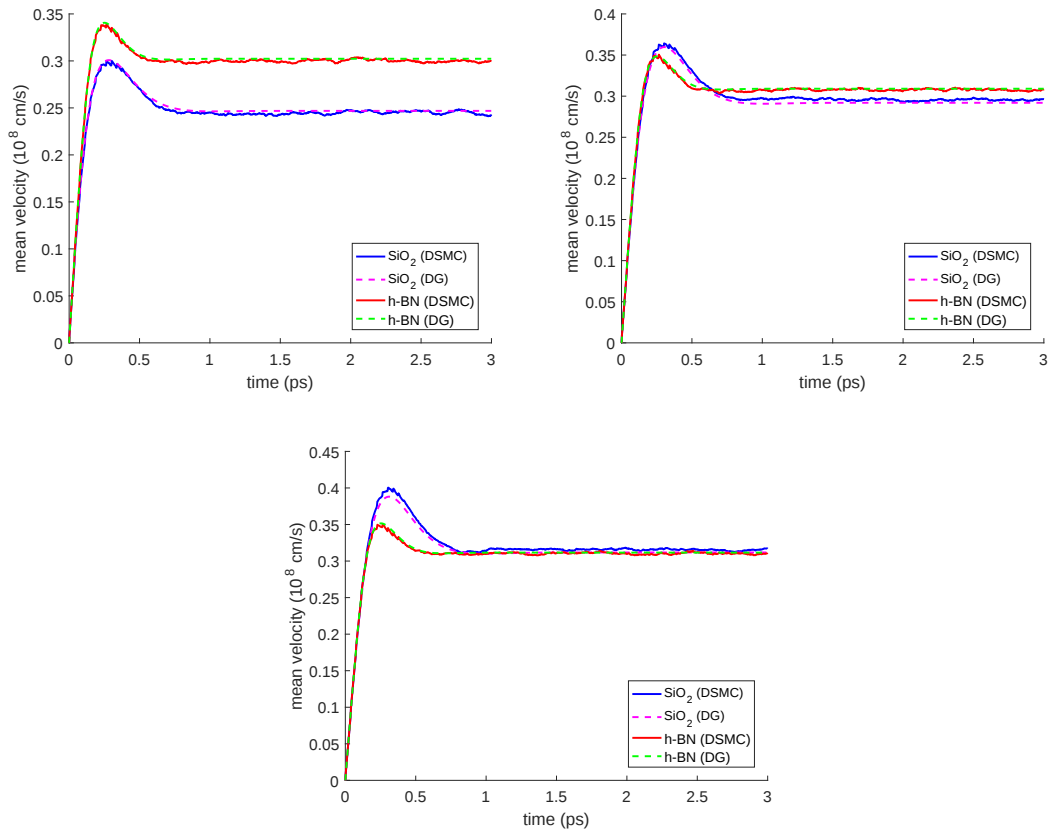


FIGURE 4.9: Comparison of the average velocity versus time for d equal to 0 nm (top-left), 0.5 nm (top-right), 1 nm (bottom) in the case of an applied electric field of 10 kV/cm and Fermi energy $\varepsilon_F = 0.4$ eV. Both the results obtained by using the DSMC and the DG method are reported.

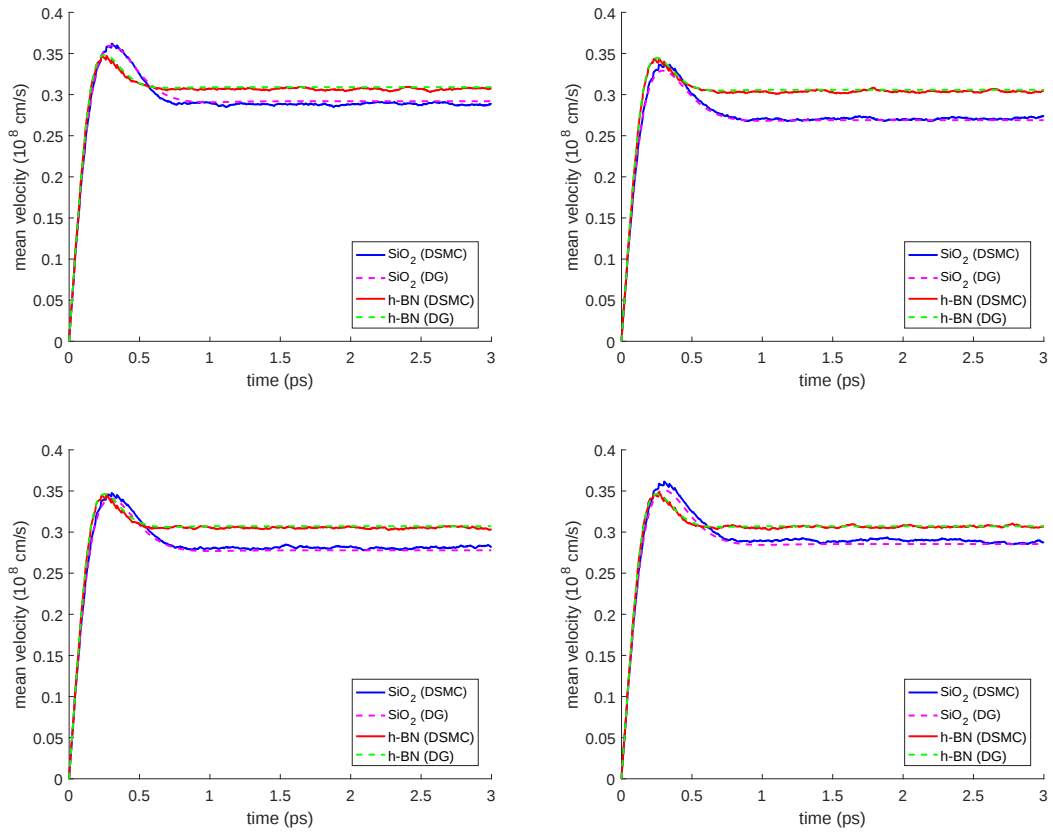


FIGURE 4.10: Comparison of the average velocity versus time in the case of an applied electric field of 10 kV/cm and Fermi energy $\varepsilon_F = 0.4$ eV by considering different distribution for d : uniform (top left), $\Gamma(2, 0.5)$ (top right), $\Gamma(3, 0.5)$ (bottom left), $\Gamma(4, 0.5)$ (bottom right). In the results obtained with the DG method we have assumed d equal to the mean value of the corresponding distribution rescaled by the factor 0.2.

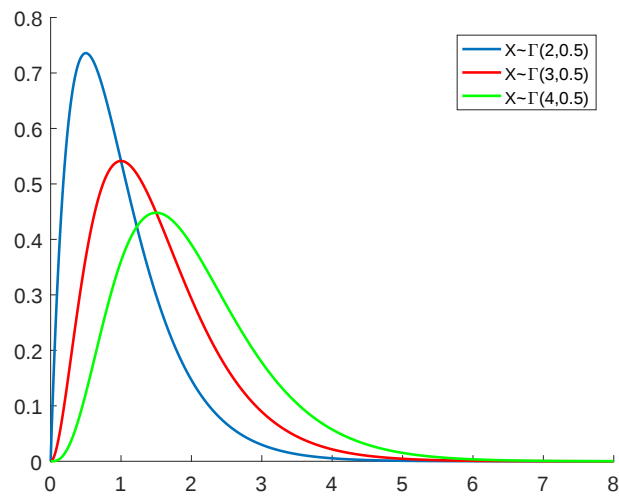


FIGURE 4.11: Plot of the $\Gamma(\alpha, \lambda)$ distribution with $\lambda = 0.5$ and $\alpha = 2, 3, 4$. Note that the probability to generate a number greater than 5 is practically zero.

4.3 The mobility model in the case of monolayer graphene between two layers of oxide substrate

To determine the analytical expression of the mobility in the case of graphene placed between two layers of oxide (SiO_2) substrate we adopt the same approach in [81]. By using a numerical scheme based on Discontinuous Galerkin (DG) method, we solve the Boltzmann equations for charge transport in graphene and get the characteristic curves; from these the expressions of the mobilities are fitted. At variance with similar procedures based on DSMC results, the numerical solutions obtained by the DG method are free from statistical noise. This is particularly important for an accurate evaluation of the low field mobility. Here all the details relative to the DG scheme are skipped. The interested reader is referred to [25, 63]. We only mention that there have been included electron-phonon scatterings, electron-impurities scatterings and scattering with the remote phonon of the substrate, taking into account both intra and inter-band interactions (see Section 1.3). Even in this situation, if the distance d between the graphene layer and the remote impurities present in the substrate is high enough, about 1 nm, the influence of the remote impurities reduces and the results are similar to the suspended case.

First we determine the low field mobility μ_0 , which is defined as

$$\mu_0(n) = \lim_{E \rightarrow 0} \mu_n(E, n). \quad (4.10)$$

For several values of charge density corresponding to a Fermi level between 0 eV and 0.4 eV, the low field mobility is extrapolated, by a linear regression model, computing the mobility at different low values of electric field, between $0.0005 \text{ V}/\mu\text{m}$ and $0.0025 \text{ V}/\mu\text{m}$, by using the values of the currents obtained by the direct solution of the Boltzmann equation with the DG method, as explained in [81]. One observes (see Figure 4.1) that in the case of graphene on substrate the low field mobility behaviour versus the density (or equivalently the Fermi energy) is similar to the suspended one but with two main differences: the peak is a minimum and for high values of density the mobility still increases.

On the basis of the previous considerations, we assume the following trial expression

$$\mu_0(n) = \tilde{\mu}_1 - \tilde{\mu}_0 \frac{\exp\left(-\frac{(\log(n/n_{ref}) - m)^2}{2\sigma^2}\right)}{\sqrt{2\pi}\sigma n/n_{ref}} \left(a \left(\frac{n}{n_{ref}} \right)^2 + b \frac{n}{n_{ref}} + c \right), \quad (4.11)$$

where $\tilde{\mu}_0$, $\tilde{\mu}_1$, n_{ref} , m , σ , a , b and c are fitting parameters. The behaviour is the same

for holes on account of the symmetry between the hole and electron distributions. We

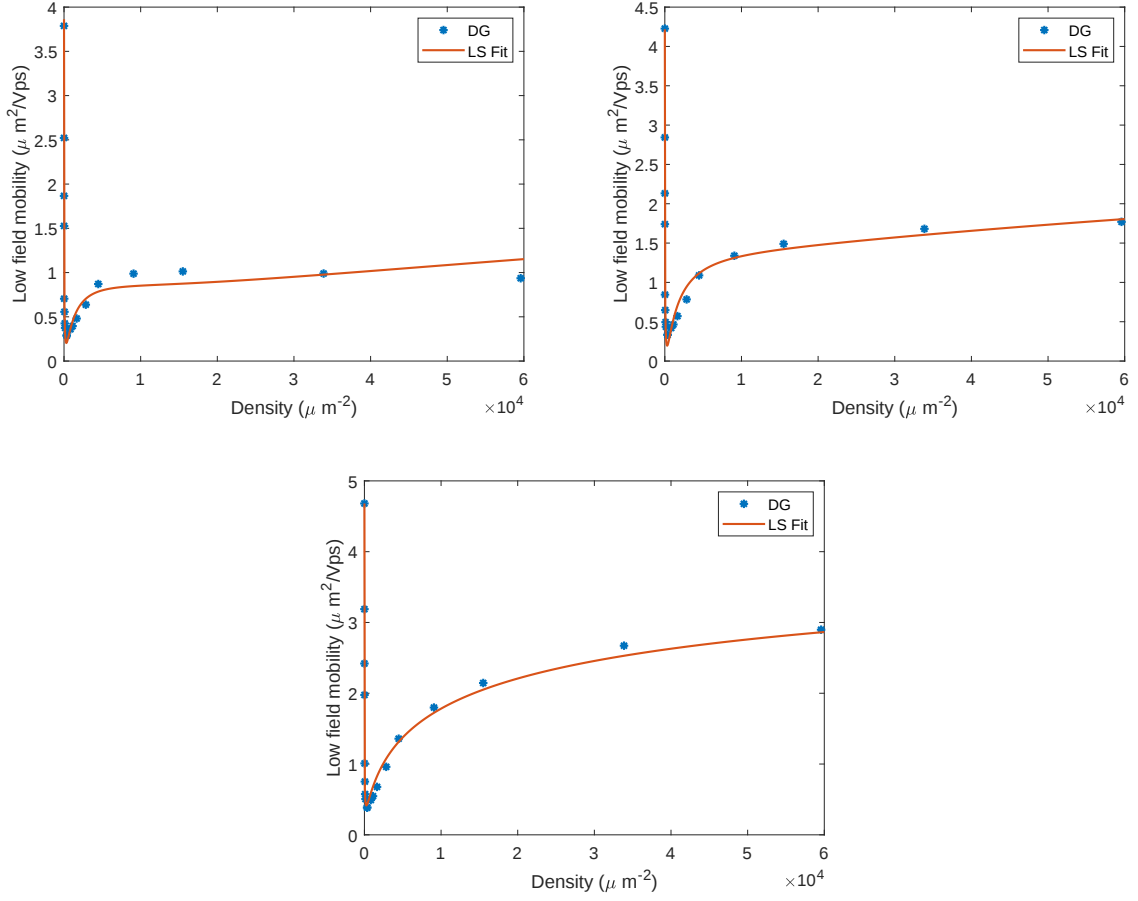


FIGURE 4.12: Comparison between the low field mobility simulated with the DG method and the fitted one at distance $d = 0\text{ nm}$ (top left), $d = 0.5\text{ nm}$ (top right) and $d = 1\text{ nm}$ (bottom).

have estimated the parameters by means of the least squares method. The obtained values are reported in Table 4.6. Observe that at variance with [24] a double strip of oxide has been considered. This enhances the effects of the remote impurities with respect to the case of graphene on a single substrate .

As second step, we include the electric field dependence by proposing a modified version of the model described in Ref. [81],[62]

$$\mu(E, n) = \frac{\mu_0(n) + \tilde{\mu} \left(\frac{E}{E_{ref}} \right)^{\beta_1}}{1 + \left(\frac{E}{E_{ref}} \right)^{\beta_2} + \gamma \left(\frac{E}{E_{ref}} \right)^{\beta_3}}, \quad (4.12)$$

where E_{ref} , $\tilde{\mu}$, β_1 , β_2 , β_3 and γ are fitting parameters. In this case we evaluated the mobility by means of the DG results of the transport equations at different densities, corresponding to the Fermi levels of 0.1 eV, 0.2 eV, 0.3 eV, 0.4 eV, 0.5 eV and for a range

	$\tilde{\mu}_0$ ($\mu m^2/Vps$)	$\tilde{\mu}_1$ ($\mu m^2/Vps$)	n_{ref} (μm^{-2})	m	σ
$d = 0$ nm	2.235e-02	3.871e+00	2.206e+02	1.406e-01	2.247e+00
$d = 0.5$ nm	2.978e-01	4.223e+00	3.769e+02	-2.838e-01	2.216e+00
$d = 1$ nm	4.300e-04	4.743e+00	7.019e+07	5.542e+00	4.255e+00

	a	b	c
$d = 0$ nm	4.548e+01	8.332e+02	4.324e+01
$d = 0.5$ nm	4.820e+00	6.834e+01	2.372e+00
$d = 1$ nm	-2.8538e+03	2.4217e+03	3.202e+03

TABLE 4.6: Estimated parameters for the low field mobility.

of electric fields between 0.025 V/ μm and 1 V/ μm . The distance d has set 0.5 nm which seems physically appropriate.

For each value of the electron density we calculate the coefficients E_{ref} , β_1 , β_2 , β_3 , γ and $\tilde{\mu}$ by means of least square method. We obtaining the data reported in Tab. 4.7. Then in each interval $[n_i, n_{i+1}]$ a third degree polynomial interpolation has

n	E_{ref}	β_1	β_2	β_3	γ	$\tilde{\mu}$
4471.0 ($\varepsilon_F = 0.1$ eV)	0.05265	1.034	2.135	1.059	14.53	12.78
15500.0 ($\varepsilon_F = 0.2$ eV)	0.02126	0.4615	1.584	0.4276	21.77	33.3
33877.0 ($\varepsilon_F = 0.3$ eV)	0.1096	1.344	2.52	1.457	4.595	6.579
59588.0 ($\varepsilon_F = 0.4$ eV)	0.1776	2.304	3.099	1.335	1.395	1.251
92644.0 ($\varepsilon_F = 0.5$ eV)	0.05047	1.988	2.661	1.109	0.8816	1.915

TABLE 4.7: High field mobility parameters at $d = 0.5$ nm. For each density the relative Fermi energy is also indicated.

been adopted for the parameters E_{ref} , β_1 , β_2 , β_3 , γ and $\tilde{\mu}$

$$a_3(n - n_i)^3 + a_2(n - n_i)^2 + a_1(n - n_i) + a_0, \quad i = 1, \dots, 4 \quad (4.13)$$

The coefficients are listed in Tab.s 4.8 - 4.13.

a_3	a_2	a_1	a_0
-2.182e-16	2.629e-10	-5.719e-6	0.05265
-1.823e-14	5.968e-10	0	0.02126
-2.756e-15	3.882e-11	3.47e-6	0.1096
1.78e-16	-1.222e-10	0	0.1776

TABLE 4.8: Coefficients in the interpolation of E_{ref} .

A comparison between fitted and simulated values of mobility models and corresponding current densities are plotted in Figure 4.13.

a_3	a_2	a_1	a_0
1.183e-13	2.095e-9	-8.94e-5	1.034
-1.594e-13	5.544e-9	0	0.4615
-4.898e-14	1.066e-9	4.232e-5	1.344
-8.768e-15	1.034e-25	0	2.304

TABLE 4.9: Coefficients in the interpolation of β_1 .

a_3	a_2	a_1	a_0
9.934e-14	2.337e-9	-8.781e-5	2.135
-2.075e-13	6.586e-9	0	1.584
-1.983e-14	1.441e-10	3.192e-5	2.52
-6.294e-15	-1.919e-10	0	3.099

TABLE 4.10: Coefficients in the interpolation of β_2 .

a_3	a_2	a_1	a_0
1.211e-13	2.517e-9	-9.972e-5	1.059
-3.322e-13	9.152e-9	0	0.4276
5.897e-15	-3.353e-10	0	1.457
9.58e-17	-4.249e-11	-5.548e-6	1.335

TABLE 4.11: Coefficients in the interpolation of β_3 .

a_3	a_2	a_1	a_0
-4.867e-13	-4.876e-8	0.001253	14.53
4.863e-12	-1.402e-7	0	21.77
-1.364e-14	4.433e-9	-0.0002295	4.595
2.301e-15	3.172e-10	-2.852e-5	1.395

TABLE 4.12: Coefficients in the interpolation of γ .

a_3	a_2	a_1	a_0
-5.07e-12	-5.689e-8	0.003105	12.78
7.506e-12	-2.171e-7	0	33.3
5.425e-14	5.269e-9	-0.0003785	6.579
1.837e-14	0	0	1.251

TABLE 4.13: Coefficients in the interpolation of $\tilde{\mu}$.

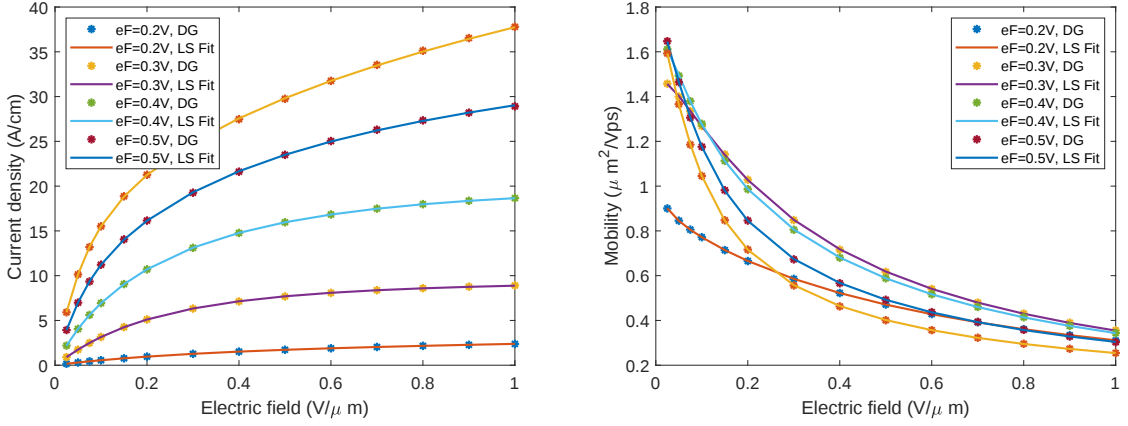


FIGURE 4.13: On the left the comparison of the simulated and fitted current densities for several values of the Fermi energy. On the right comparison between the mobility simulated with the DG method and the fitted one for several values of the Fermi energy.

4.4 A full coupled drift-diffusion-Poisson simulation of a GFET

Metal Oxide Semiconductor Field Effect Transistor (MOSFET) is the backbone of the modern integrated circuits. In the case when the active area is made of traditional materials like, for example, silicon or gallium arsenide, a lot of analysis and simulations have been performed in order to optimize the design. Lately a great attention has been devoted to graphene on account of its peculiar features, and in particular, from the point of view of nano-electronics, for the high electrical conductivity. It is highly tempting to try to replace the traditional semiconductors with graphene in the active area of electron devices like the MOSFETs. In fact as quoted in [95] "Graphene has changed from being the exclusive domain of condensed-matter physicists to being explored by those in the electron-device community. In particular, graphene-based transistors have developed rapidly and are now considered an option for post-silicon electronics. However, many details about the potential performance of graphene transistors in real applications remain unclear."

Device engineers devote considerable effort to developing transistor designs in which short-channel effects are suppressed and series resistances are minimized. Scaling theory predicts that a FET with a thin barrier and a thin gate-controlled region will be robust against short-channel effects down to very short gate lengths. The possibility of having channels that are just one atomic layer thick is perhaps the most attractive feature of graphene for its use in transistors. Main drawbacks of a large-area single monolayer graphene are the zero gap and, for graphene on substrate, the degradation

of the mobility. Therefore accurate simulation are warranted for the set up of a viable graphene field effect transistor.

A standard mathematical model is given by a drift-diffusion-Poisson system. Usually the GFETs are investigated by adopting reduced one dimensional models of the Poisson equation with some averaging procedure [47, 103]. Here a full two-dimensional simulation is presented.

A crucial point is the determination of the mobilities entering the drift-diffusion equations. A rather popular model is that proposed in [33]. Here a different approach is adopted. Thanks to the discontinuous Galerkin (DG) scheme developed in [89, 25, 24, 63], we have performed, for graphene on a substrate, an extensive numerical simulation based on the semiclassical Boltzmann equations, including electron-phonon scatterings, electron-impurities scatterings and scattering with the remote phonon of the substrate, taking into account both intra and inter-band scatterings. From the numerical solutions of the semiclassical Boltzmann equation a model for the mobility functions has been deduced, similarly to what already done in [62] and in [81] in the case of suspended monolayer graphene.

Note that the solutions furnished by deterministic methods, like DG ones, are noise free and allow us to determine in an accurate way the low field mobility. Similar results obtained starting from the DSMC results are quite questionable because of the intrinsic statistical noise.

In this section we describe the mathematical model and present the numerical results of the simulation of a top-gated GFET by means of both the mobility model of Section 4.3 and the one of Ref. [33]. It is confirmed the critical issue of the GFET related to the restricted current off region due to the zero gap which produces a relevant current due to the minority charges when the gate voltage decreases below a threshold value. It is likely that other type of GFET must be tried to improve the performance of a device made of a single layer graphene.

4.4.1 Mathematical model

For our purpose let us consider a section of the device like that depicted in Fig. 4.14. The active zone is made of a single layer of graphene which is between two strips of insulator, both of them being SiO_2 . The source and drain contacts are directly above the graphene. The two gate contacts (up and down) are attached to the oxide.

On the considered section we solve a 2D Poisson equation, assuming that the charge is concentrated on the volume occupied by the atoms composing the graphene layer. Accordingly, the surface charge density of graphene is supposed to be spanned on its thickness which experimental measurements refer between 0.4 nm and 1.7 nm [97].

In order to simulate the current flowing in the channel we adopt the 1D bipolar drift-diffusion model, coupled to the Poisson equation for the electrostatic potential in the whole section. A special attention is required by the initial carrier density profiles that have to be determined compatibly with the electric potential, leading to a nonlinear Poisson equation as will be discussed in the following.

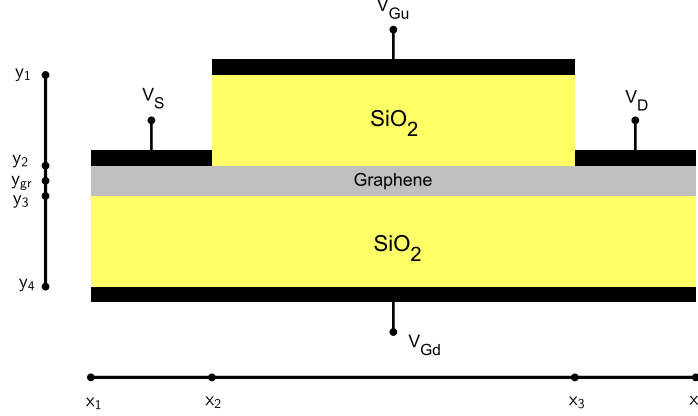


FIGURE 4.14: Schematic representation of a GMOSFET.

The bipolar drift-diffusion model is adopted in $[x_2, x_3] \times \{y_{gr}\}$ and it reads

$$\frac{\partial n}{\partial t} - \frac{\partial}{\partial x} \left(\mu_n U_T \frac{\partial n}{\partial x} - n \mu_n \frac{\partial \phi}{\partial x} \right) = 0, \quad (4.14)$$

$$\frac{\partial p}{\partial t} + \frac{\partial}{\partial x} \left(-\mu_p U_T \frac{\partial p}{\partial x} - p \mu_p \frac{\partial \phi}{\partial x} \right) = 0, \quad (4.15)$$

where $n(t, x)$, $p(t, x)$ are the electron and hole densities in graphene respectively, $U_T = k_B T / e$ is the thermal voltage, being e the positive elementary charge, k_B is the Boltzmann constant, T is the lattice temperature (kept constant). The functions $\mu_n(x)$ and $\mu_p(x)$ are the mobilities for electrons and holes respectively and $\phi(x, y)$ is the electric potential, here evaluated on $y = y_{gr}$, y_{gr} being the y -coordinate of the graphene sheet (see Fig. 4.14). The generation and recombination terms are set equal to zero[81]. Indeed, this relation is strictly valid at the steady state but here will be assumed during the transient as well. We expect that the stationary solutions is not affected by such an approximation. A typical behaviour of the total generation and recombination term versus time, obtained with the DG method in [89, 25, 24, 63], is reported in Fig. 4.15. Initially there is the creation of electron-hole pairs with a rate which depends on the Fermi energy but after a transient of several tens of picoseconds the Pauli principle prevents the formation of new electron-hole pairs and one has a stationary regime with zero generation-recombination term.

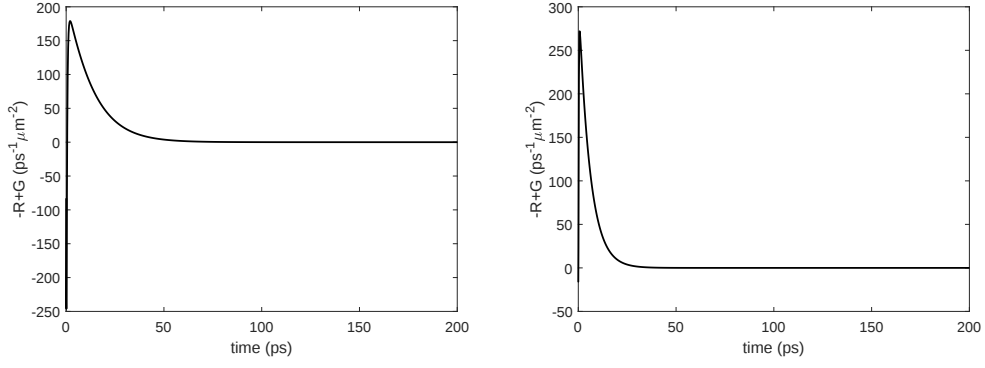


FIGURE 4.15: Production term $-R + G$, with R and G recombination and generation respectively, versus time in homogeneous graphene with zero Fermi energy (left) and with a Fermi energy 0.1 eV (right). In both cases an applied electric field of 5 kV/cm has been considered. A similar behaviour is found by varying the Fermi energy and the electric field.

The system is solved in the interval $[x_2, x_3]$ augmented with Dirichlet boundary conditions

$$n|_{x=x_2} = n_0, \quad n|_{x=x_3} = n_L, \quad p|_{x=x_2} = p_0, \quad p|_{x=x_3} = p_L.$$

How to fix the values n_0, n_L, p_0, p_L depends on the modelling of the contacts and will be explained below.

The electric potential solves the 2D Poisson equation

$$\nabla \cdot (\epsilon \nabla \phi) = h(x, y), \quad (4.16)$$

where

$$h(x, y) = \begin{cases} e(n(x) - p(x))/t_{gr} & \text{if } y = y_{gr}, \quad x \in [x_2, x_3] \\ 0 & \text{otherwise} \end{cases}$$

and ϵ is given by

$$\epsilon(x, y) = \begin{cases} \epsilon_{gr} & \text{if } y = y_{gr} \\ \epsilon_{ox} & \text{if } y \neq y_{gr} \end{cases}$$

Here $\epsilon_{gr} = 3.3\epsilon_0$ and $\epsilon_{ox} = 3.6\epsilon_0$ are the dielectric constants of the graphene and oxide (SiO₂) respectively, ϵ_0 being the dielectric constant in the vacuum. t_{gr} is the width of the graphene layer which is assumed to be 1 nm. The charge in the graphene layer is considered as distributed in the volume enclosed by the parallelepiped of base the area of the graphene and height t_{gr} . Recall that n and p are areal densities. Dirichlet conditions are imposed on the gate contacts and homogeneous Neumann conditions on the external oxide edges. A major issue is to model the source and drain regions where

metal and graphene touch. We assume that source and drain are thermal bath charge reservoirs following a Fermi-Dirac distribution. The injection of charges is determined by a work function W_F . Indeed it depends on the specific material the contacts are made of. We set $W_F = 0.25V$ which is appropriate for Cu; in fact, this is within the experimentally observed range of 0.20 eV [37] and 0.30 eV [106].

As summary the following boundary conditions for the electric potential are imposed

$$\begin{aligned}
 \phi &= W_F & \text{at } y = y_{gr}, x \in [x_1, x_2] \\
 \phi &= W_F + V_b & \text{at } y = y_{gr}, x \in [x_3, x_4] \\
 \phi &= W_F + V_{G_u} & \text{at } y = y_1, x \in [x_2, x_3] \\
 \phi &= W_F + V_{G_d} & \text{at } y = y_4, x \in [x_1, x_4] \\
 \nabla_\nu \phi &= 0 & \text{at the remaining part of the boundary.}
 \end{aligned} \tag{4.17}$$

V_b is the bias voltage, V_{G_u} is the upper gate-source potential, V_{G_d} is the down gate-source potential. We have denoted by ∇_ν the normal derivative.

In standard doped semiconductors the initial carrier densities are equal to the doping profile and the boundary conditions are given by the charge neutrality and the Ohmic (alternatively Shottcky) contact conditions. On the contrary in graphene a sort of doping is induced if an electric field perpendicular to the layer is applied [53] due to a shift of the Fermi energy. Assuming thermal equilibrium, the initial carrier densities are related to the electric potential by

$$\begin{aligned}
 n_0(x) &= \frac{2}{(2\pi)^2} \int_{\mathbb{R}^2} f_{FD}(\mathbf{k}; e\phi(x, y_{gr})) d\mathbf{k}, & x \in [x_2, x_3], \\
 p_0(x) &= \frac{2}{(2\pi)^2} \int_{\mathbb{R}^2} f_{FD}(\mathbf{k}; -e\phi(x, y_{gr})) d\mathbf{k}, & x \in [x_2, x_3],
 \end{aligned} \tag{4.18}$$

being f_{FD} the Fermi-Dirac distribution

$$f_{FD}(\mathbf{k}, \varepsilon_F) = \frac{1}{1 + \exp\left(\frac{\varepsilon(\mathbf{k}) - \varepsilon_F}{k_B T}\right)}, \tag{4.19}$$

where ε_F is the Fermi level (in pristine graphene $\varepsilon_F = 0$), $\varepsilon(\mathbf{k})$ is the graphene dispersion relation (strictly valid around the Dirac points)

$$\varepsilon(\mathbf{k}) = \hbar v_F |\mathbf{k}|, \tag{4.20}$$

which is the same for electrons and holes (see [44, 52]), $\hbar$ is the reduced Planck constant and v_F is the Fermi velocity. The crystal momentum of electrons and holes is assumed to vary all over $\mathbb{R}^2$.

Therefore boundary conditions at the contacts are given by

$$\begin{cases} n_0(x_2) = \frac{2}{(2\pi)^2} \int \frac{1}{1 + \exp\left(\frac{\varepsilon(\mathbf{k}) - eW_F}{k_B T}\right)} d\mathbf{k}, \\ p_0(x_2) = \frac{2}{(2\pi)^2} \int \frac{1}{1 + \exp\left(\frac{\varepsilon(\mathbf{k}) + eW_F}{k_B T}\right)} d\mathbf{k}, \end{cases} \quad (4.21)$$

$$\begin{cases} n_0(x_3) = \frac{2}{(2\pi)^2} \int \frac{1}{1 + \exp\left(\frac{\varepsilon(\mathbf{k}) - eW_F - eV_b}{k_B T}\right)} d\mathbf{k}, \\ p_0(x_3) = \frac{2}{(2\pi)^2} \int \frac{1}{1 + \exp\left(\frac{\varepsilon(\mathbf{k}) + eW_F + eV_b}{k_B T}\right)} d\mathbf{k}. \end{cases} \quad (4.22)$$

In the second relation the definition of hole distribution has been taken into account along with the fact that the energy band is a even function of the modulus of the wave vector.

Altogether, in order to get the initial density profile as function of the electric potential, we must solve the following nonlinear Poisson equation

$$\nabla \cdot (\epsilon \nabla \phi) = g(\phi), \quad (4.23)$$

where

$$g(\phi(x, y)) = \begin{cases} e(n_0(\phi(x, y)) - p_0(\phi(x, y))) / t_{gr} & \text{if } y = y_{gr}, x \in [x_2, x_3] \\ 0 & \text{otherwise} \end{cases} \quad (4.24)$$

augmented with the boundary conditions (4.17).

4.4.2 Numerical method for the drift-diffusion-Poisson system

To solve the drift-diffusion-Poisson system we employ the strategy already discussed in Section 2.3, based on the Scharfetter-Gummel scheme together with the standard finite difference scheme for the Poisson equation.

Since the initial condition is given by the non linear Poisson equation (4.23), in order to get it we adopt the following iterative scheme.

1. Set an initial guess $n^{(1)} = n_{ini}(x)$, $p^{(1)} = p_{ini}(x)$ and get $\phi^{(1)}$ through (4.16).
2. For each $r > 1$:

(a) solve the Poisson equation

$$\nabla \cdot (\epsilon \nabla \phi^{(r+1)}) = g(\phi^{(r)})$$

to get $\phi^{(r+1)}$;

(b) find $n^{(r+1)}(x)$, $p^{(r+1)}(x)$ by using (4.18);

3. Iterate step 2 until convergence.

In order to improve the convergence, the Poisson equation is solved by means of the Gummel method (see [40]) adding a term in the diagonal elements of the scheme

$$\begin{aligned} & \frac{\epsilon_{i+\frac{1}{2},j} \phi_{i+1,j}^r - (\epsilon_{i+\frac{1}{2},j} + \epsilon_{i-\frac{1}{2},j}) \phi_{i,j}^r + \epsilon_{i-\frac{1}{2},j} \phi_{i-1,j}^r}{\Delta x^2} \\ & + \frac{\epsilon_{i,j+\frac{1}{2}} \phi_{i,j+1}^r - (\epsilon_{i,j+\frac{1}{2}} + \epsilon_{i,j-\frac{1}{2}}) \phi_{i,j}^r + \epsilon_{i,j-\frac{1}{2}} \phi_{i,j-1}^r}{\Delta y^2} \\ & - \frac{n_i^{r-1} + p_i^{r-1}}{\epsilon_0 t_{gr} r_B T} \phi_{i,j}^r = g_{i,j}^{r-1} - \frac{n_i^{r-1} + p_i^{r-1}}{\epsilon_0 t_{gr} r_B T} \phi_{i,j}^{r-1}. \end{aligned}$$

4.4.3 Numerical results for the G-MOSFET with the mobility based on the Boltzmann equation

The GFET of Fig. 4.14 has been intensively simulated. We have set the length 100 nm, the width of the lower and upper oxide (SiO₂) 10 nm. The source and drain contacts are long 25 nm. The two gate potentials are considered as equal.

We considered a mesh of 40 grid points along the x -direction. Along the y -axis, between the gate contacts we have 23 grid points while in the region below source and drain we have 12 grid points. In the graphene layer a single row of 40 nodes has been employed. The steady state is reached in about one ps.

In order to get the solution the following strategy has been adopted:

1. first the Poisson equation is solved by keeping the charge in the graphene layer equal to n_0 and p_0 for electron and holes, respectively;
2. then the nonlinear Poisson problem (4.23)-(4.24) is solved with the iterative scheme described in Sec.4.4.2, by taking as initial guess the solution of step 1;
3. once the initial data for the electron and hole density have been determined the full transient drift-diffusion-Poisson system is solved

The electrostatic potential is plotted in Fig. 4.16. The characteristic curves are shown in Figs 4.17, 4.18. The behaviour is qualitatively similar to other results existing in

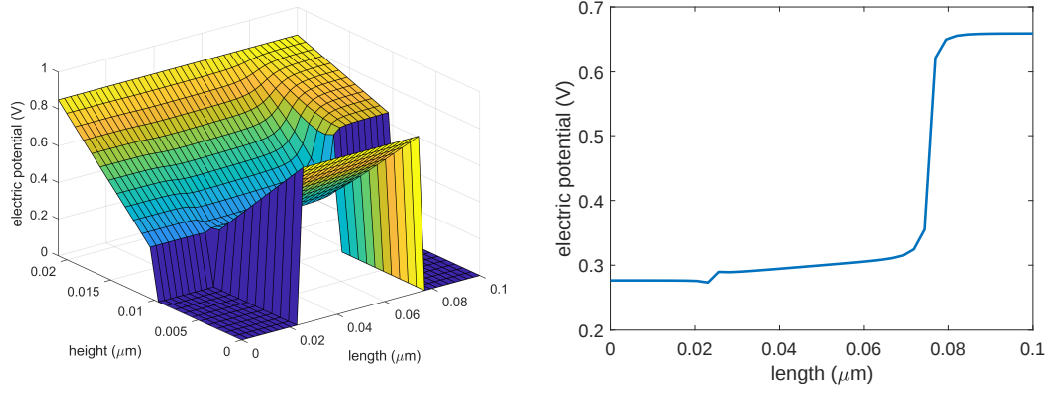


FIGURE 4.16: 2D electrostatic potential (left) in the case $V_G = 0.6$ V, $V_b = 0.4$ V. The upper gate is at $y = 0$. Similar results have been obtained in the other cases. The electric potential along the graphene is plotted on the left.

the literature. Note the presence of kinks which have been already discussed in [70]. Moreover, as shown by Fig. 4.18, apart the cases of low gate voltage, the current is not always a monotone function of the bias voltage showing in some range the effects of negative differential mobility. However, at variance with other results, see for example the review in [95], apparently the characteristic curve as function of the source-drain voltage present a sort of saturation effect.

Above the inversion gate voltage (about -0.5 V) the majority carriers are the electrons while below the inversion voltage the majority carriers are the holes. The critical issue is the difficulty of fixing the off state which requires an accurate calibration of the gate voltages, although an acceptable current-on over current-off ratio as shown in Figs 4.17 (left).

When the gate voltage changes sign, the current due to the minority charge is triggered. As a consequence the GFET presents only a limited off region around the gate voltage -0.5 V. Even with the new mobility model and a simulation of the full 2D Poisson equation, we have a further confirmation of this feature which makes GFET not the optimal device for post-silicon nanoscale electron technology. Other attempts, like multi-layer GFETs or, probably better, double gate GFETs must be tested.

4.4.4 Numerical results for the G-MOSFET with the mobility of Dorgan et al.

The simulated device is again the one depicted in Fig. 4.14. The length is 100 nm. The width of the lower and upper oxide (SiO_2) is 10 nm. The source and drain contacts are long 25 nm. The mobility model is the one of Ref. [33], already introduced in Section 4.1.2. The two gate potentials are set as equal. At the metallic contacts the total voltage

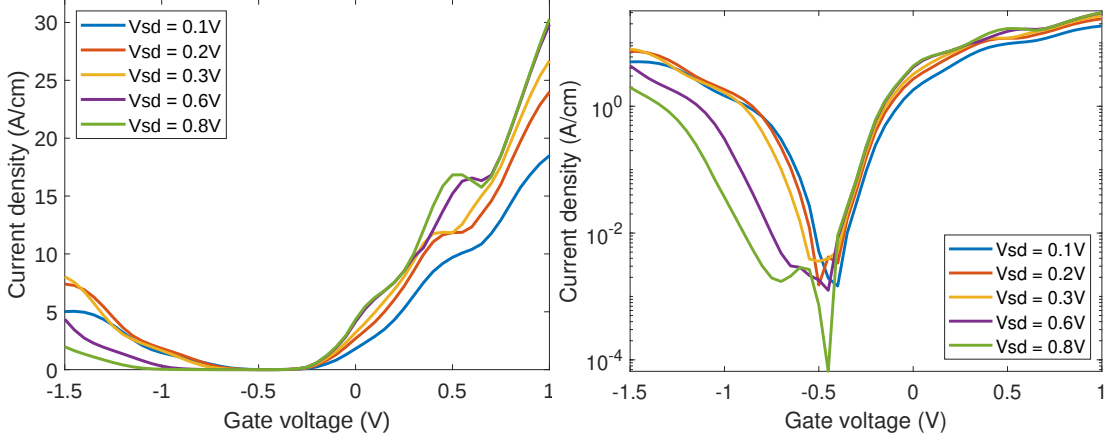


FIGURE 4.17: Total current versus gate voltage at fixed bias in a linear scale (left) and a semi-logarithmic scale (right).

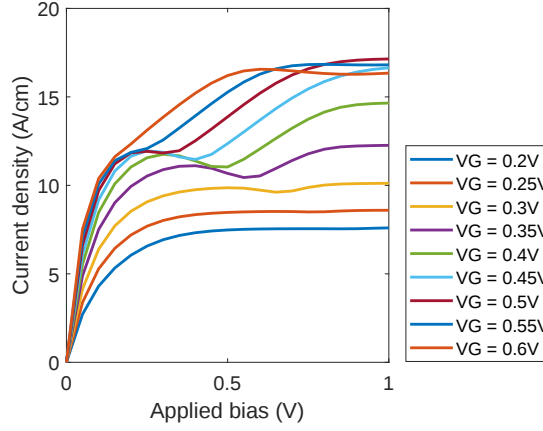


FIGURE 4.18: Total current versus bias at fixed gate voltages.

includes also the work function which depends on the specific material the contacts are made of. Different values of the work function will be considered in the simulations.

In Fig. 4.19 the shape of the electrical potential is plotted when the gate-source potential is 0.6 V and the source-drain-potential is 0.3 V, with a work function of 0.25 V. The impurity charge is neglected. Similar results are obtained in the other cases.

Fig. 4.20 (left) shows the characteristic curves of current versus gate voltage with work function equal to 0 V for several values of the source-drain voltage, neglecting the impurities. In Fig. 4.20 (right) the current versus gate voltage are plotted as in Fig. 4.20 (left), including also the presence of an impurity density of $3.5 \times 10^3 \mu\text{m}^{-2}$, for several values of the gate voltage. The presence of the impurities produces a small degradation of the current. The crucial issue is that the range of gate voltage where the current is off is bounded at variance with traditional semiconductors. This is due to the gapless nature of monolayer graphene. As a consequence, a fine tuning of the gate voltage is required to have an acceptable field effect transistor and in this respect accurate simulations are needed.

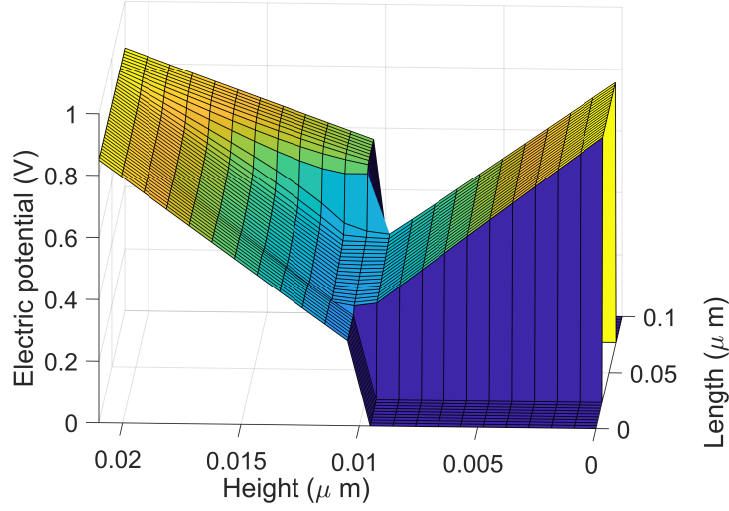


FIGURE 4.19: Electrostatic potential when the gate-source potential is 0.6 V and the source-drain-potential is 0.3 V. The work function potential is 0.25 V.

In Fig. 4.21 the previous characteristic curves are shown by considering a work function of 0.25 V. Again the presence of the impurities leads only to a small degradation of the current. Note that above the inversion voltage (0.25 V) the majority carriers are the electrons while below the inversion voltage the majority carriers are the holes. The behaviour of the current is very different from the traditional semiconductors like Si or GaAs on account of the zero gap in the energy band. The major issue is the difficulty of fixing the off state which requires an accurate calibration of the voltage. To complete the analysis, in Fig. 4.22 we show the current versus the source-drain voltage for several gate-source voltages with a work function at the graphene-metal interface equal to 0.25 V.

4.5 Conclusions

In Section 1 and 3, new mobility models for charge transport in graphene have been obtained by resorting to an extensive numerical simulation of the Boltzmann transport equations with a DG method. Both the cases of suspended graphene and graphene on substrate have been considered. Comparisons with other models present in the literature show a considerable improvement. Further developments could include the effects of crystal heating and quantum effects in the mobility models. Although the subject is still in an early stage, attempts in this direction can be found in [67, 30] regarding the thermal influence on the electric performance, and in [72, 59] regarding the inclusion of quantum corrections.

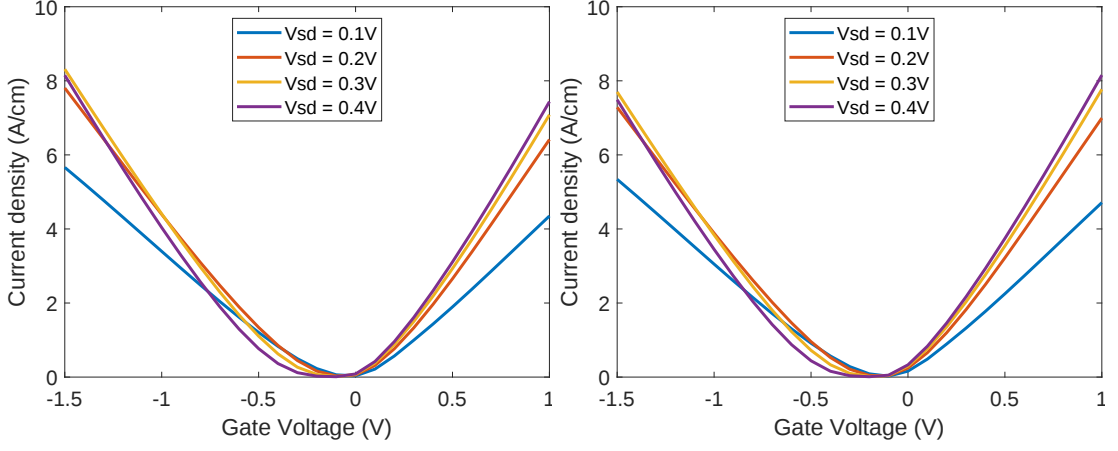


FIGURE 4.20: Current versus gate voltage with a work function at the graphene-metal interface equal to 0V without impurities (left) and including an impurity density of $3.5 \times 10^3 \mu\text{m}^{-2}$ (right).

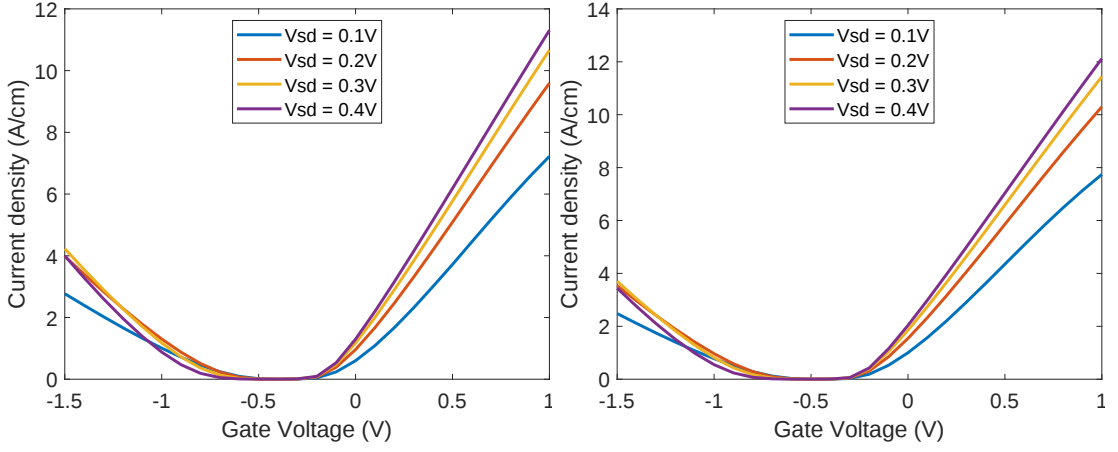


FIGURE 4.21: Current versus gate voltage with a work function at the graphene-metal interface equal to 0.25V without impurities (left) and including an impurity density of $3.5 \times 10^3 \mu\text{m}^{-2}$ (right).

In Section 2, an analysis of the high-field mobility has been performed for graphene on a substrate by a new DSMC approach, which properly takes into account the Pauli exclusion principle. The same substrates as in [42] have been considered but including the more accurate model for the charge-impurities scattering (see [43]). Moreover, also the random distribution of the depth of the impurities implanted in the oxide has been taken into account and described with several theoretical probability distributions. The differences among the average velocities for the considered substrates are in agreement with the expected effects and confirm a degradation of the mobility. As already found out in [42] for the low field mobility, h-BN reveals a better substrate than SiO₂, because it produces a smaller degradation also in the high-field mobility.

In Section 3, top-gated GFETs have been simulated and the characteristic curves

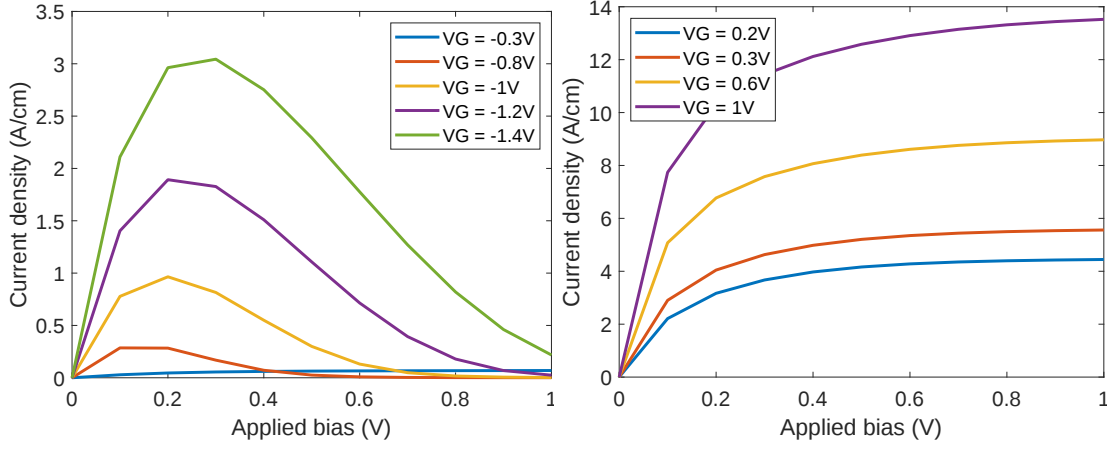


FIGURE 4.22: Current versus source-drain voltage with a work function at the graphene-metal interface equal to 0.25 V including an impurity density of $3.5 \times 10^3 \mu\text{m}^{-2}$. Negative (left) and positive (right) gate-source voltages are considered.

have shown. The current-voltage curves present a behaviour different from that of devices made of classical semiconductors, like Si or GaAs, because of the zero gap in monolayer graphene. A full numerical solution of a drift-diffusion-Poisson model have been included. First we have been adopted mobility expression of ref. [33], next the mobilities have been deduced from the direct solution of the Boltzmann equations for charge transport in graphene by a DG method, as explained in Section 3. The results confirm the main features of such a devices. In particular the limited range of gate-source voltages for the current-off state.

Chapter 5

Classical-quantum drift-diffusion model of charge transport in graphene

Very peculiar quantum phenomena were predicted and experimentally demonstrated in graphene, such as Klein paradox (see [51, 108]) and Veselago lensing (see [20, 54]). They offer interesting opportunities to nano-electronics and opto-electronics.

The above mentioned phenomena are related to the chiral nature of electrons in graphene [19] and take place in the presence of steps or barriers of the electric potential, that can be realized by suitable electric gates or doping profiles.

In [9, 10] a hybrid model has been proposed. It couples a thin *active* quantum region, containing the rapid potential variations, with two *classical* regions, where the transport regime is diffusive and incoherent. The coupling is firstly described at the kinetic level, where the classical-quantum matching is more natural, and then the diffusive limit is analyzed by means of the Hilbert expansion method. In [59] a hydrodynamical model based on the maximum entropy principle (MEP), which includes also quantum effects, has been formulated.

In this chapter we introduce some preliminary results, in preprint form [8], concerning the numerical solutions of the model proposed in [9, 10]. In Section 5.1 we show how to get the coupling system in the two dimensional case; in Section 5.2 we propose a simplified one dimensional and unipolar system, in order to simulate the device of ref. [108].

The results of this chapter has been obtained during two visiting periods at the Institut de Mathématiques de Toulouse, Université Toulouse III - Paul Sabatier, under the supervision of Prof. C. Negulescu, and one visiting period at the Dipartimento di Matematica e Informatica “Ulisse Dini”, Università degli Studi di Firenze, under the supervision of Prof. Luigi Barletti.

5.1 Model description

First we briefly recall that in [10] the following results have been obtained. Assume that a graphene sheet is described by the coordinates $x = (x, y)$ and that a potential step, or barrier, is localized at $x = 0$. More precisely, we assume that the electric potential has the form

$$V(x) + U(x, y),$$

where $V(x)$ represents the step/barrier profile, which is assumed to have variations localized around $x = 0$ and to take constant values V^1 and V^2 at the left and at the right, respectively. The “smooth” part of the potential, $U(x, y)$ is assumed to vary on a much larger (macroscopic space scale). Accordingly, the graphene sheet is divided in two “classical” regions ($x < 0$ and $x > 0$), where the charge transport is described by the drift-diffusion equation

$$\operatorname{div} j_s = 0, \quad j_s = -\frac{\tau v_F^2}{2} [\nabla n_s + s\beta n_0 \phi_1(A_s) \nabla U]. \quad (5.1)$$

Here, $n_s(x, y)$ denote the densities of electrons ($s = +1$) and holes ($s = -1$), τ is the typical electron-phonon collision time, and the constants n_0 and β are given by

$$\beta = \frac{1}{k_B T}, \quad n_0 = \frac{2\pi}{(2\pi\hbar v_F \beta)^2} = \frac{(k_B T)^2}{2\pi\hbar^2 v_F^2}$$

(where, as usual, k_B is the Boltzmann constant, T is the temperature of the phonon bath, v_F is the Fermi velocity). Moreover,

$$\phi_k(z) := \frac{1}{\Gamma(k)} \int_0^\infty \frac{t^{k-1}}{e^{t-z} + 1} dt$$

is the Fermi integral of order k , and A_s are the chemical potentials, related to the densities by

$$A_s = A(n_s) := \phi_2^{-1}\left(\frac{n_s}{n_0}\right). \quad (5.2)$$

The right and left regions are linked through diffusive transmission conditions (DTC) which, at first order in τ read as follows:

$$sA(n_s^1 + \tau n_s^{1,\infty}) = s'A(n_{s'}^2 + \tau n_{s'}^{2,\infty}) + \beta\delta V. \quad (5.3)$$

Here, $\delta V = V^2 - V^1$ is the overall potential variation across the barrier, the upper index $i = 1, 2$ denotes the left and right sides with respect to the barrier, namely

$$n_s^1 = \lim_{x \rightarrow 0^-} n_s, \quad n_{s'}^2 = \lim_{x \rightarrow 0^+} n_{s'}.$$

The relation (5.3) is assumed to hold for all couples of left and right electron/hole labels, $s = \pm 1, s' = \pm 1$, such that the conservation of energy

$$sc|\mathbf{p}| = s'c|\mathbf{p}'| + \delta V, \quad (5.4)$$

is satisfied for some left and right pseudomomentum $\mathbf{p} = (p_x, p_y) \in \mathbb{R}^2$ and $\mathbf{p}' = (p'_x, p'_y) \in \mathbb{R}^2$. The possible couples (s, s') are:

$$\begin{aligned} & (++) , (+, -) , (-, -) && \text{if } \delta V > 0, \\ & (++) , (-, -) && \text{if } \delta V = 0, \\ & (++) , (-, +) , (-, -) && \text{if } \delta V < 0. \end{aligned}$$

The four constants $n_s^{i,\infty}$ (possibly functions of y), $s = \pm 1, i = 1, 2$, are the most important parameters in the theory. They are obtained as the asymptotic values of the electron/hole left/right densities of the solutions of the four Milne-like equations

$$\frac{p_x}{|\mathbf{p}|} \frac{\partial f_s^i}{\partial x} = L_s^i \langle f_s^i \rangle - f_{s'}^i, \quad (-1)^i x > 0, \quad (5.5)$$

for the boundary layer correctors f_s^i , where

$$\langle f_s^i \rangle := \frac{1}{(2\pi\hbar)^2} \int_{\mathbb{R}^2} f_s^i d\mathbf{p}$$

and

$$L_s^i(\mathbf{p}) := \frac{1}{n_0 \phi_1(A(n_s^i))} \frac{e^{\beta v_F |\mathbf{p}| - A(n_s^i)}}{(e^{\beta v_F |\mathbf{p}| - A(n_s^i)} + 1)^2}. \quad (5.6)$$

The four Milne equations are coupled at $x = 0$ by the non-homogeneous quantum transmission conditions

$$\begin{cases} f_s^1(p_x) - f_s^1(-p_x) + T_{s'}^2(\mathbf{p}') \left(f_s^1(-p_x) - ss' f_{s'}^2(p'_x) \right) = h_s^1(\mathbf{p}), & p_x, p'_x < 0, \\ f_{s'}^2(p'_x) - f_{s'}^2(-p'_x) + T_s^1(\mathbf{p}) \left(f_{s'}^2(-p_x) - ss' f_s^1(p'_x) \right) = h_{s'}^2(\mathbf{p}'), & p'_x, p_x > 0, \end{cases} \quad (5.7)$$

where $T_s^i(\mathbf{p})$ is the transmission coefficient (which can be obtained by solving the stationary Schrödinger equation for the potential V) and

$$\begin{cases} h_s^1(\mathbf{p}) := G_s^1(p_x) - G_s^1(-p_x) + T_{s'}^2(\mathbf{p}') \left(G_s^1(-p_x) - ss' G_{s'}^2(p'_x) \right), & p_x, p'_x < 0, \\ h_{s'}^2(\mathbf{p}') := G_{s'}^2(p'_x) - G_{s'}^2(-p'_x) + T_s^1(\mathbf{p}) \left(G_{s'}^2(-p'_x) - ss' G_s^1(p'_x) \right), & p'_x, p_x > 0, \end{cases} \quad (5.8)$$

with

$$G_s^i(\mathbf{p}) = \frac{2}{v_F^2} L_s^i(\mathbf{p}) \frac{\mathbf{p}}{|\mathbf{p}|} \cdot \mathbf{j}_s^i.$$

It can be proven that, asymptotically far from the interface $x = 0$, the solution has the form

$$f_s^i(x, y, \mathbf{p}) \approx L_s^i(\mathbf{p}) n_s^{i,\infty}(y), \quad \text{as } x \rightarrow (-1)^{i,\infty}$$

where $n_s^{i,\infty}$ are the parameters eq. (5.3) depends on. We notice that all the information coming from quantum mechanics is codified in these four parameters.

In the Maxwell-Boltzmann limit ($\beta v_F |\mathbf{p}| \gg A(n)$), the model outlined above takes a simplified form: the drift-diffusion equation (5.1) becomes

$$\text{div} \mathbf{j}_s = 0, \quad \mathbf{j}_s = -\frac{\tau v_F^2}{2} [\nabla n_s + s \beta n_s \nabla U], \quad (5.9)$$

the DTC (5.3) becomes

$$\left(\frac{n_s^1 + \tau n_s^{1,\infty}}{n_0} \right)^s = \left(\frac{n_{s'}^2 + \tau n_{s'}^{2,\infty}}{n_0} \right)^{s'} e^{\beta \delta V}, \quad (5.10)$$

and the distribution (5.6) becomes a Maxwellian-like distribution

$$L_s^i(\mathbf{p}) \approx M(\mathbf{p}) := \frac{e^{-\beta v_F |\mathbf{p}|}}{n_0}. \quad (5.11)$$

Note, in particular, that M does not depend on n_s^i while L_s^i does.

The DTC (5.3) or (5.10) must be complemented with the current conservation relations

$$\begin{cases} j_{+,x}^1 - j_{-,x}^1 = j_{+,x}^2 - j_{-,x}^2 & \text{if } \delta V > 0, \\ \left. \begin{aligned} j_{+,x}^1 &= j_{+,x'}^2 \\ j_{-,x}^1 &= j_{-,x}^2 \end{aligned} \right\} & \text{if } \delta V = 0, \end{cases}$$

(where $j_{s,x}^1$ and $j_{s,x}^2$ denote, respectively, the left and right values of the x -component of the drift-diffusion current $\mathbf{j}_s$ at $x = 0$).

We finally remark that, still at first-order in τ , the DTC (5.3) are equivalent to the following relation

$$sA(n_s^1) - s'A(n_{s'}^2) - \beta\delta V = \frac{\tau}{n_0} \left(\frac{s'n_{s'}^{2,\infty}}{c_{s'}^2} - \frac{s n_s^{1,\infty}}{c_s^1} \right) \quad (5.12)$$

where we put

$$c_s^i := \phi_1(A(n_s^1))$$

and we recall that

$$A(n) = \phi_2^{-1} \left(\frac{n}{n_0} \right).$$

5.1.1 Application to a prototype graphene device

We consider a device constituted by a graphene sheet and represented by the rectangle $(x, y) \in (-L, L) \times (-l, l)$. At boundaries $x = -L$ and $x = L$ there are placed two metallic Ohmic contacts and at boundaries $y = -l$ and $y = l$ there are insulators. We suppose that an external electric field ∇U is applied and a steep potential with amplitude δV is concentrated at $x = 0$. We remark that in this chapter all potentials are indeed energies ($\delta V = e\tilde{V}$, $U = e\tilde{U}$ with $\tilde{V}$ and $\tilde{U}$ physical potentials). Let us split the domain in two classical regions

$$\Omega^1 = (-L, 0) \times (-l, l), \quad \Omega^2 = (0, L) \times (-l, l)$$

and a quantum interface at $x = 0$.

If we define as n_s the charge concentration for electrons (+) or holes (-), the resulting hybrid diffusive-quantum model reads as follows:

- in the semiclassical region $\Omega^1 \cup \Omega^2$

$$\begin{cases} \nabla \cdot \mathbf{j}_s = 0 \\ \mathbf{j}_s = -(\nabla n_s + s\beta n_s \nabla U) \end{cases} \quad (5.13)$$

where $\beta = 1/k_B T$

- at the Ohmic boundary $x = \pm L$

$$n_s = n_s^{\pm L} \quad (5.14)$$

- at the insulating boundary $y = \pm l$

$$j_{s,y} = 0 \quad (5.15)$$

- across the quantum interface $x = 0$

$$\begin{cases} n_+^1 - e^{\beta\delta V} n_+^2 = \tau (e^{\beta\delta V} n_+^{2,\infty} - n_+^{1,\infty}) \\ n_+^1 n_-^2 + \tau (n_+^1 n_-^{2,\infty} + n_-^2 n_+^{1,\infty}) = e^{\beta\delta V} (n_0)^2 \\ n_-^1 - e^{-\beta\delta V} n_-^2 = \tau (e^{-\beta\delta V} n_-^{2,\infty} - n_-^{1,\infty}) \\ j_{+,x}^1 - j_{-,x}^1 = j_{+,x}^2 - j_{-,x}^2 \end{cases} \quad (5.16)$$

where τ is the typical collision time and $n_0 = 2\pi/(hc\beta)^2$ with $\beta = 1/k_B T$ is the intrinsic graphene concentration being c the Fermi velocity and h the Planck constant.

Finally the current densities are given by

$$\mathbf{J}_s = -e\tau \frac{c^2}{2} \mathbf{j}_s.$$

If we make the following assumptions on the electric potential energy

1. $V = V(x)$ depends only on the variable x (which implies that it conserves p_y);
2. $V(x) \rightarrow 0$ on the left and $V(x) \rightarrow \delta V$ on the right of a *quantum strip* around $x = 0$, having a vanishing strip on a macroscopic length scale,

then we obtain a scattering problem, providing us the transmission and reflection coefficients. We denote by $T_s^i(\mathbf{p})$ and $R_s^i(\mathbf{p})$ the transmission and reflection coefficients from the left ($i = 1$) to the right ($i = 2$). They satisfy the following properties

1. unitarity: $T_s^i(\mathbf{p}) \geq 0$ and $R_s^i(\mathbf{p}) \geq 0$, with $T_s^i(\mathbf{p}) + R_s^i(\mathbf{p}) = 1$;
2. energy-dependence: $T_s^i(\mathbf{p})$ and $R_s^i(\mathbf{p})$ depend on $\mathbf{p}$ and s only through the energy $sc|\mathbf{p}|$;
3. reciprocity: $T_s^1(\mathbf{p}) = T_{s'}^2(\mathbf{p}')$ whenever the conservation of energy $sc|\mathbf{p}| = s'c|\mathbf{p}'| + \delta V$ holds.

For example, for a potential step of height δV the transmission coefficient for an electron incident from the left, with energy $E = sc|\mathbf{p}|$, to the right, with energy $E' = s'c|\mathbf{p}'| = sc|\mathbf{p}| - \delta V$, is given by

$$T_s^1(\mathbf{p}) = \begin{cases} \frac{2ss' \cos(\phi) \cos(\theta)}{1 + ss' \cos(\phi + \theta)} & \text{if } |E \sin(\phi)| < |E - \delta V| \\ 0 & \text{otherwise} \end{cases} \quad (5.17)$$

where $\phi \in (-\frac{\pi}{2}, \frac{\pi}{2})$ is the incidence angle and $\theta \in (-\frac{\pi}{2}, \frac{\pi}{2})$ is the transmission angle. Since $\mathbf{p} = (p_x, p_y)$ the energy condition

$$|sc|\mathbf{p}| \sin(\phi)| < |sc|\mathbf{p}| - \delta V|$$

becomes

$$|p_y| < |s|\mathbf{p}| - \delta V/c|$$

and therefore the incidence angle determines the quantities

$$\begin{aligned} \cos(\phi) &= \frac{p_x}{|\mathbf{p}|}, \quad p_x > 0 \\ \sin(\phi) &= \frac{p_y}{|\mathbf{p}|}. \end{aligned}$$

In order to find explicit expressions for the transmission coefficient we need to distinguish two cases with respect to s . If $s = +$ we have two possibilities: if $E > \delta V$ then $s' = +$ else $s' = -$. In this second case the electron is replaced by an hole and its wave-vector is opposite. This leads to the expressions

$$\sin(\theta) = \frac{s'cp_y}{c|\mathbf{p}| - \delta V}, \quad \cos(\theta) = s'\sqrt{1 - \sin^2(\theta)}$$

obtaining finally

$$T_+^1(\mathbf{p}) = \begin{cases} \frac{2 \cos(\phi) \cos(\theta)}{1 + \cos(\phi + \theta)} & \text{if } |p_y| < ||\mathbf{p}| - \delta V/c| \text{ and } |\mathbf{p}| > \delta V/c \\ -\frac{2 \cos(\phi) \cos(\theta)}{1 - \cos(\phi + \theta)} & \text{if } |p_y| < ||\mathbf{p}| - \delta V/c| \text{ and } |\mathbf{p}| < \delta V/c \\ 0 & \text{otherwise} \end{cases} \quad (5.18)$$

If $s = -$ the only one possibility is $s' = -$ and an hole is still an hole and the transmission angle is given by [10]

$$\sin(\theta) = \frac{cp_y}{c|\mathbf{p}| + \delta V}, \quad \cos(\theta) = \sqrt{1 - \sin^2(\theta)}$$

and explicitly we have

$$T_-^1(\mathbf{p}) = \begin{cases} \frac{2 \cos(\phi) \cos(\theta)}{1 + \cos(\phi + \theta)} & \text{if } |p_y| < ||\mathbf{p}| + \delta V/c| \\ 0 & \text{otherwise} \end{cases} \quad (5.19)$$

For $i = 2$, because of the various symmetries of the problem, we have

$$T_+^2(\mathbf{p}) = T_-^1(\mathbf{p}) \quad \text{and} \quad T_-^2(\mathbf{p}) = T_+^1(\mathbf{p}).$$

5.1.2 Milne problem

Across the quantum interface the quantities $n_s^{i,\infty}$, appearing in (5.16), can be obtained in the following way. Let us consider the Milne problem

$$\begin{cases} \mu \frac{\partial \theta_s^i}{\partial \xi} = F'_{n_s^i} \langle \theta_s^i \rangle - \theta_s^i, & (-1)^i \xi > 0 \\ \theta_{s,\text{in}}^i - \mathcal{K}^i(\theta_{s,\text{out}}^i, \theta_{s,\text{out}}^j) = G_{s,\text{in}}^i - \mathcal{K}^i(G_{s,\text{out}}^i, G_{s,\text{out}}^j), & \xi = 0 \end{cases} \quad (5.20)$$

where

$$F'_{n_s^i}(\mathbf{p}) = \frac{F_{n_s^i}(\mathbf{p})^2 e^{\beta c |\mathbf{p}| - A(n_s^i)}}{n_0 \phi_1(A(n_s^i))} \quad (5.21)$$

with

- $F_{n_s^i}(\mathbf{p}) = \frac{1}{e^{\beta c |\mathbf{p}| - A(n_s^i)} + 1}$;
- $A(n_s^i) = \phi_2^{-1} \left(\frac{n_s^i}{n_0} \right)$;
- $\phi_k(z) = \frac{1}{\Gamma(k)} \int_0^{+\infty} \frac{t^{k-1}}{e^{t-z} + 1} dt$,

and

$$\mathcal{K}^i(f_{s,\text{out}}^i, f_{s,\text{out}}^j)(\mathbf{p}) = R_s^i(\mathbf{p}) f_{s,\text{out}}^i(\sim \mathbf{p}) + ss' T_{s'}^j(\mathbf{p}') f_{s',\text{out}}^j(\mathbf{p}'), \quad (5.22)$$

with $\sim \mathbf{p} = (-p_x, p_y)$. To prove this we consider the operator

$$\mathcal{B}^i(f_{s,\text{out}}^i, f_{s,\text{out}}^j)(\mathbf{p}) = R_s^i(\mathbf{p}) f_{s,\text{out}}^i(\sim \mathbf{p}) + T_s^j(\mathbf{p}') \left(ss' f_{s,\text{out}}^j(\mathbf{p}') + \epsilon_{ss'} \right) \quad (5.23)$$

where

$$\epsilon_{ss'} = \begin{cases} 0, & \text{if } s = s' \\ 1, & \text{if } s \neq s' \end{cases} \quad (5.24)$$

and apply it to $(f + g)_{s,\text{out}}^i$ obtaining

$$\begin{aligned}
 \mathcal{B}^i((f + g)_{s,\text{out}}^i (f + g)_{s,\text{out}}^j)(\mathbf{p}) &= R_s^i(\mathbf{p})(f + g)_{s,\text{out}}^i(\sim \mathbf{p}) + T_s^j(\mathbf{p}') \\
 &\quad \times \left(ss'(f + g)_{s,\text{out}}^j(\mathbf{p}') + \epsilon_{ss'} \right) \\
 &= R_s^i(\mathbf{p})f_{s,\text{out}}^i(\sim \mathbf{p}) + R_s^i(\mathbf{p})g_{s,\text{out}}^i(\sim \mathbf{p}) \\
 &\quad + T_s^j(\mathbf{p}') \left(ss'f_{s,\text{out}}^j(\mathbf{p}') + ss'g_{s,\text{out}}^j(\mathbf{p}') + \epsilon_{ss'} \right) \\
 &= R_s^i(\mathbf{p})f_{s,\text{out}}^i(\sim \mathbf{p}) + T_s^j(\mathbf{p}') \left(ss'f_{s,\text{out}}^j(\mathbf{p}') + \epsilon_{ss'} \right) \\
 &\quad + R_s^i(\mathbf{p})g_{s,\text{out}}^i(\sim \mathbf{p}) + ss'T_s^j(\mathbf{p}')g_{s,\text{out}}^j(\mathbf{p}') \\
 &= \mathcal{B}^i(f_{s,\text{out}}^i, f_{s,\text{out}}^j)(\mathbf{p}) + \mathcal{K}^i(g_{s,\text{out}}^i, g_{s,\text{out}}^j)(\mathbf{p}).
 \end{aligned}$$

We remark that quantities $\mathbf{p}$, $\mathbf{p}'$, s and s' are related by

$$s'c|\mathbf{p}'| = sc|\mathbf{p}| + (-1)^i \delta V \quad (5.25)$$

(expressing the conservation of energy) and the left and right densities at interface are constrained by

$$sA(n_s^i) = s'A(n_{s'}^j) + (-1)^j \beta \delta V. \quad (5.26)$$

Now let us substitute (5.22) in (5.20)₂ and consider the relation $R_s^i(\mathbf{p}) = 1 - T_s^i(\mathbf{p})$ obtaining

$$\theta_{s,\text{in}}^i - (1 - T_s^i(\mathbf{p}))\theta_{s,\text{out}}^i(\sim \mathbf{p}) - ss'T_{s'}^j(\mathbf{p}')\theta_{s',\text{out}}^j(\mathbf{p}') = h_s^i(\mathbf{p}), \quad (5.27)$$

where

$$h_s^i(\mathbf{p}) = G_{s,\text{in}}^i - \mathcal{K}^i(G_{s,\text{out}}^i, G_{s,\text{out}}^j). \quad (5.28)$$

The next step is to introduce some approximation techniques for the solution of the Milne problem. The so-called Albedo approximation consists in finding solutions of the form

$$\theta_{s,\text{out}}^i = L^s(\mathbf{p})\rho_s^i \quad (-1)^i p_x < 0$$

where ρ_s^i are unknown outflow densities satisfying a condition of vanishing total flux at interface. We shall adopt a further simplification, named Marshak approximation, which consists in assuming

$$\rho_s^i = n_s^{i,\infty}$$

The meaning of Marshak approximation is that one identifies the outflow density with the asymptotic density, which is indeed reached exponentially fast away from the interface. The interested reader is referred to [32] for further information. From equation

(5.21) we have that

$$F'_{n_s^i}(\sim \mathbf{p}) = F'_{n_s^i}(\mathbf{p}), \quad (5.29)$$

then $L_s^i(\sim \mathbf{p}) = L_s^i(\mathbf{p})$ and by using reciprocity property, $T_{s'}^j(\mathbf{p}') = T_s^i(\mathbf{p})$, we obtain

$$\theta_{s,\text{in}}^i - L_s^i(\mathbf{p})\rho_s^i + T_s^i(\mathbf{p})[L_s^i(\mathbf{p})\rho_s^i - ss'L_{s'}^j(\mathbf{p}')\rho_{s'}^j] = h_s^i(\mathbf{p}). \quad (5.30)$$

Now we consider (5.21) and by using (5.25), (5.26) we can calculate

$$\begin{aligned} \phi_1(A(n_s^i))F'_{n_s^i}(\mathbf{p}) &= \frac{1}{n_0}F_{n_s^i}(\mathbf{p})^2 e^{\beta c|\mathbf{p}| - A(n_s^i)} = \frac{1}{n_0} \frac{e^{\beta c|\mathbf{p}| - A(n_s^i)}}{(e^{\beta c|\mathbf{p}| - A(n_s^i)} + 1)^2} = \\ &= \frac{1}{n_0} \frac{\exp\left(\beta\left(\frac{s'}{s}c|\mathbf{p}'| - \frac{(-1)^i}{s}\delta V\right) - \frac{s'}{s}A(n_{s'}^j) - \frac{(-1)^j}{s}\beta\delta V\right)}{\left(\exp\left(\beta\left(\frac{s'}{s}c|\mathbf{p}'| - \frac{(-1)^i}{s}\delta V\right) - \frac{s'}{s}A(n_{s'}^j) - \frac{(-1)^j}{s}\beta\delta V\right) + 1\right)^2} = \\ &= \frac{1}{n_0} \frac{\exp\left(\frac{s'}{s}\left(\beta c|\mathbf{p}'| - A(n_{s'}^j)\right)\right)}{\left(\exp\left(\frac{s'}{s}\left(\beta c|\mathbf{p}'| - A(n_{s'}^j)\right)\right) + 1\right)^2} = \\ &= \frac{1}{n_0} \frac{\exp\left(\beta c|\mathbf{p}'| - A(n_{s'}^j)\right)}{\left(\exp\left(\beta c|\mathbf{p}'| - A(n_{s'}^j)\right) + 1\right)^2} = \\ &= \frac{1}{n_0}F_{n_{s'}^j}(\mathbf{p}')^2 e^{\beta c|\mathbf{p}'| - A(n_{s'}^j)} = \phi_1(A(n_{s'}^j))F'_{n_{s'}^j}(\mathbf{p}'), \end{aligned}$$

where the terms with δV disappear because $i \neq j$ and also s'/s because

$$\frac{e^h}{(e^h + 1)^2} = \frac{e^{-h}}{(e^{-h} + 1)^2}.$$

This leads to the relation

$$c_s^i L_s^i(\mathbf{p}) = c_{s'}^j L_{s'}^j(\mathbf{p}') \quad (5.31)$$

being $c_s^i := \phi_1(A(n_s^i)) = \phi_1(\phi_2^{-1}(n_s^i/n_0))$. By using this relation in (5.30) we have finally

$$\theta_{s,\text{in}}^i - L_s^i(\mathbf{p})\rho_s^i + T_s^i(\mathbf{p})L_s^i(\mathbf{p}) \left[\rho_s^i - ss' \frac{c_s^i}{c_{s'}^j} \rho_{s'}^j \right] = h_s^i(\mathbf{p}), \quad (5.32)$$

that holds on $\mathbb{R}_{\text{in}}^{2,i} := \{\mathbf{p} \in \mathbb{R}^2 \mid (-1)^i p_x > 0\}$. Now we multiply (5.32) by $\mu = \mu(\mathbf{p}) = cp_x/|\mathbf{p}|$ and integrate over $\mathbb{R}_{\text{in}}^{2,i}$ obtaining

$$\int_{\mathbb{R}_{\text{in}}^{2,i}} \theta_{s,\text{in}}^i \mu d\mathbf{p} - \int_{\mathbb{R}_{\text{in}}^{2,i}} L_s^i(\mathbf{p})\rho_s^i \mu d\mathbf{p} + \int_{\mathbb{R}_{\text{in}}^{2,i}} T_s^i(\mathbf{p})L_s^i(\mathbf{p}) \left[\rho_s^i - ss' \frac{c_s^i}{c_{s'}^j} \rho_{s'}^j \right] \mu d\mathbf{p} = \int_{\mathbb{R}_{\text{in}}^{2,i}} h_s^i(\mathbf{p}) \mu d\mathbf{p}. \quad (5.33)$$

By performing the change of variables $p_x \rightarrow -p_x$ on the second integral we obtain

$$\int_{\mathbb{R}_{\text{in}}^{2,i}} \theta_{s,\text{in}}^i \mu d\mathbf{p} - \int_{\mathbb{R}_{\text{in}}^{2,i}} L_s^i(\mathbf{p}) \rho_s^i \mu d\mathbf{p} = \int_{\mathbb{R}_{\text{in}}^{2,i}} \theta_{s,\text{in}}^i \mu d\mathbf{p} + \int_{\mathbb{R}_{\text{out}}^2} L_s^i(\mathbf{p}) \rho_s^i \mu d\mathbf{p} = 0, \quad (5.34)$$

because both the Albedo and the Marshak approximations are constructed so that the x -flow of θ_s^i at $\xi = 0$ vanishes. Then we have

$$\int_{\mathbb{R}_{\text{in}}^{2,i}} T_s^i(\mathbf{p}) L_s^i(\mathbf{p}) \left[\rho_s^i - s s' \frac{c_s^i}{c_{s'}^j} \rho_{s'}^j \right] \mu d\mathbf{p} = H_{s'}^i, \quad (5.35)$$

where

$$H_s^i = \int_{\mathbb{R}_{\text{in}}^{2,i}} h_s^i(\mathbf{p}) \mu d\mathbf{p}. \quad (5.36)$$

Let us write these cases explicitly

$$\begin{aligned} & \int_{\{\mathbf{p} \in \mathbb{R}^2 | p_x < 0, c|\mathbf{p}| > \delta V\}} T_+^1(\mathbf{p}) L_+^1(\mathbf{p}) \left[\rho_+^1 - \frac{c_+^1}{c_+^2} \rho_+^2 \right] \mu d\mathbf{p} \\ & + \int_{\{\mathbf{p} \in \mathbb{R}^2 | p_x < 0, c|\mathbf{p}| < \delta V\}} T_+^1(\mathbf{p}) L_+^1(\mathbf{p}) \left[\rho_+^1 + \frac{c_+^1}{c_-^2} \rho_-^2 \right] \mu d\mathbf{p} = H_+^1 \quad (i=1, j=2, s=+, s'=\pm) \\ & \int_{\{\mathbf{p} \in \mathbb{R}^2 | p_x < 0\}} T_-^1(\mathbf{p}) L_-^1(\mathbf{p}) \left[\rho_-^1 - \frac{c_-^1}{c_-^2} \rho_-^2 \right] \mu d\mathbf{p} = H_-^1 \quad (i=1, j=2, s=-, s'=-) \\ & \int_{\{\mathbf{p} \in \mathbb{R}^2 | p_x > 0\}} T_+^2(\mathbf{p}) L_+^2(\mathbf{p}) \left[\rho_+^2 - \frac{c_+^2}{c_+^1} \rho_+^1 \right] \mu d\mathbf{p} = H_+^2 \quad (i=2, j=1, s=+, s'=+) \\ & \int_{\{\mathbf{p} \in \mathbb{R}^2 | p_x > 0, c|\mathbf{p}| > \delta V\}} T_-^2(\mathbf{p}) L_-^2(\mathbf{p}) \left[\rho_-^2 + \frac{c_-^2}{c_+^1} \rho_+^1 \right] \mu d\mathbf{p} \\ & + \int_{\{\mathbf{p} \in \mathbb{R}^2 | p_x > 0, c|\mathbf{p}| < \delta V\}} T_-^2(\mathbf{p}) L_-^2(\mathbf{p}) \left[\rho_-^2 - \frac{c_-^2}{c_-^1} \rho_-^1 \right] \mu d\mathbf{p} = H_-^2 \quad (i=2, j=1, s=-, s'=\pm) \end{aligned}$$

Next we choose different unknowns by setting

$$\begin{cases} X_{++} = \rho_+^1 - \frac{c_+^1}{c_+^2} \rho_+^2 \\ X_{+-} = c_-^2 \rho_+^1 + c_+^1 \rho_-^2 \\ X_{--} = \rho_-^1 - \frac{c_-^1}{c_-^2} \rho_-^2 \end{cases} \quad (5.37)$$

and then we can rewrite the previous equations as

$$X_{++} \int_{\{\mathbf{p} \in \mathbb{R}^2 | p_x < 0, c|\mathbf{p}| > \delta V\}} T_+^1(\mathbf{p}) L_+^1(\mathbf{p}) \mu d\mathbf{p} \quad (5.38)$$

$$+ X_{+-} \int_{\{\mathbf{p} \in \mathbb{R}^2 | p_x < 0, c|\mathbf{p}| < \delta V\}} \frac{1}{c_-^2} T_+^1(\mathbf{p}) L_+^1(\mathbf{p}) \mu d\mathbf{p} = H_+^1 \quad (5.39)$$

$$X_{--} \int_{\{\mathbf{p} \in \mathbb{R}^2 | p_x < 0\}} T_-^1(\mathbf{p}) L_-^1(\mathbf{p}) \mu d\mathbf{p} = H_-^1 \quad (5.40)$$

$$- X_{++} \int_{\{\mathbf{p} \in \mathbb{R}^2 | p_x > 0\}} \frac{c_+^2}{c_+^1} T_+^2(\mathbf{p}) L_+^2(\mathbf{p}) \mu d\mathbf{p} = H_+^2 \quad (5.41)$$

$$X_{+-} \int_{\{\mathbf{p} \in \mathbb{R}^2 | p_x > 0, c|\mathbf{p}| > \delta V\}} \frac{1}{c_+^1} T_-^2(\mathbf{p}) L_-^2(\mathbf{p}) \mu d\mathbf{p} \quad (5.42)$$

$$- X_{--} \int_{\{\mathbf{p} \in \mathbb{R}^2 | p_x > 0, c|\mathbf{p}| < \delta V\}} \frac{c_-^2}{c_-^1} T_-^2(\mathbf{p}) L_-^2(\mathbf{p}) \mu d\mathbf{p} = H_-^2 \quad (5.43)$$

We consider the first three equations

$$\begin{cases} AX_{++} + BX_{+-} &= H_+^1 \\ CX_{--} &= H_-^1 \\ -DX_{++} &= H_+^2 \end{cases} \quad (5.44)$$

leading to the solution

$$\begin{cases} X_{++} = -\frac{H_+^2}{D} \\ X_{--} = \frac{H_-^1}{C} \\ X_{+-} = \frac{H_+^1}{B} + \frac{AH_+^2}{DB} \end{cases} \quad (5.45)$$

The next step is to introduce the Maxwell-Boltzmann approximation that is

$$c_s^i = \phi_1 \left(\phi_2^{-1} \left(\frac{n_s^i}{n_0} \right) \right) \approx \frac{n_s^i}{n_0}. \quad (5.46)$$

In this way we obtain

$$\begin{cases} X_{++} \approx \rho_+^1 - \frac{n_+^1}{n_+^2} \rho_+^2 \\ X_{+-} \approx \frac{n_-^2 \rho_+^1 + n_+^1 \rho_-^2}{n_0} \\ X_{--} \approx \rho_-^1 - \frac{n_-^1}{n_-^2} \rho_-^2 \end{cases} \quad (5.47)$$

and since the relations $n_s^1 = e^{s\beta\delta V} n_s^2$, with $s = \pm$, hold at order τ we have

$$\begin{cases} X_{++} \approx \rho_+^1 - e^{\beta\delta V} \rho_+^2 \\ X_{+-} \approx \frac{n_-^2 \rho_+^1 + n_+^1 \rho_-^2}{n_0} \\ X_{--} \approx \rho_-^1 - e^{-\beta\delta V} \rho_-^2 \end{cases} \quad (5.48)$$

Therefore we have

$$L_s^i(\mathbf{p}) = \frac{1}{n_0 c_s^i} \frac{e^{\beta c|\mathbf{p}| - A(n_s^i)}}{(e^{\beta c|\mathbf{p}| - A(n_s^i)} + 1)^2} \approx \frac{1}{n_0 c_s^i} \frac{e^{\beta c|\mathbf{p}| - A(n_s^i)}}{(e^{\beta c|\mathbf{p}| - A(n_s^i)})^2} = \frac{1}{n_0 c_s^i} \frac{1}{e^{\beta c|\mathbf{p}| - A(n_s^i)}} \quad (5.49)$$

$$= \frac{1}{n_0 c_s^i} e^{-\beta c|\mathbf{p}|} e^{A(n_s^i)} \approx \frac{e^{-\beta c|\mathbf{p}|}}{n_0} =: M(\mathbf{p}). \quad (5.50)$$

In this way the quantities A , B , C and D writes

$$\begin{aligned} A &= \int_{\{\mathbf{p} \in \mathbb{R}^2 | p_x < 0, c|\mathbf{p}| > \delta V\}} T_+^1(\mathbf{p}) L_+^1(\mathbf{p}) \mu d\mathbf{p} \\ &\approx \int_{\{\mathbf{p} \in \mathbb{R}^2 | p_x < 0, c|\mathbf{p}| > \delta V\}} T_+^1(\mathbf{p}) M(\mathbf{p}) \frac{c p_x}{|\mathbf{p}|} d\mathbf{p} \\ &= - \int_{\{\mathbf{p} \in \mathbb{R}^2 | p_x > 0, c|\mathbf{p}| > \delta V\}} T_+^1(\mathbf{p}) M(\mathbf{p}) \frac{c p_x}{|\mathbf{p}|} d\mathbf{p} \end{aligned}$$

$$\begin{aligned} B &= \int_{\{\mathbf{p} \in \mathbb{R}^2 | p_x < 0, c|\mathbf{p}| < \delta V\}} \frac{1}{c_-^2} T_+^1(\mathbf{p}) L_+^1(\mathbf{p}) \mu d\mathbf{p} \\ &\approx \int_{\{\mathbf{p} \in \mathbb{R}^2 | p_x < 0, c|\mathbf{p}| < \delta V\}} \frac{n_0}{n_-^2} T_+^1(\mathbf{p}) M(\mathbf{p}) \frac{c p_x}{|\mathbf{p}|} d\mathbf{p} \\ &= - \int_{\{\mathbf{p} \in \mathbb{R}^2 | p_x > 0, c|\mathbf{p}| < \delta V\}} \frac{n_0}{n_-^2} T_+^1(\mathbf{p}) M(\mathbf{p}) \frac{c p_x}{|\mathbf{p}|} d\mathbf{p} \end{aligned}$$

$$\begin{aligned} C &= \int_{\{\mathbf{p} \in \mathbb{R}^2 | p_x < 0\}} T_-^1(\mathbf{p}) L_-^1(\mathbf{p}) \mu d\mathbf{p} \\ &\approx \int_{\{\mathbf{p} \in \mathbb{R}^2 | p_x < 0\}} T_-^1(\mathbf{p}) M(\mathbf{p}) \frac{c p_x}{|\mathbf{p}|} d\mathbf{p} \\ &= - \int_{\{\mathbf{p} \in \mathbb{R}^2 | p_x > 0\}} T_-^1(\mathbf{p}) M(\mathbf{p}) \frac{c p_x}{|\mathbf{p}|} d\mathbf{p} \end{aligned}$$

$$\begin{aligned}
D &= \int_{\{\mathbf{p} \in \mathbb{R}^2 | p_x > 0\}} \frac{c_+^2}{c_+^1} T_+^2(\mathbf{p}) L_+^2(\mathbf{p}) \mu d\mathbf{p} \\
&\approx \int_{\{\mathbf{p} \in \mathbb{R}^2 | p_x > 0\}} \frac{n_+^2}{n_+^1} T_+^2(\mathbf{p}) M(\mathbf{p}) \frac{cp_x}{|\mathbf{p}|} d\mathbf{p}
\end{aligned}$$

Next we consider the source term

$$\begin{aligned}
h_s^i(\mathbf{p}) &= G_{s,\text{in}}^i - \mathcal{K}^i(G_{s,\text{out}}^i, G_{s,\text{out}}^j) \\
&= G_{s,\text{in}}^i(\mathbf{p}) - G_{s,\text{out}}^i(\sim \mathbf{p}) + T_s^i(\mathbf{p})[G_{s,\text{out}}^i(\sim \mathbf{p}) - ss' G_{s',\text{out}}^j(\mathbf{p}')]
\end{aligned}$$

where

$$G_s^i(\mathbf{p}) = cL_s^i(\mathbf{p}) \frac{\mathbf{p}}{|\mathbf{p}|} \cdot \mathbf{j}_s^i. \quad (5.51)$$

Since $\mathbf{j}_s^i$ does not depend on $\mathbf{p}$ and the quantity $L_s^i(\mathbf{p})$ only depends on $|\mathbf{p}|$ we can remove labels in and out, then we obtain

$$\begin{aligned}
h_s^i(\mathbf{p}) &= cL_s^i(\mathbf{p}) \frac{\mathbf{p}}{|\mathbf{p}|} \cdot \mathbf{j}_s^i - cL_s^i(\sim \mathbf{p}) \frac{\sim \mathbf{p}}{|\sim \mathbf{p}|} \cdot \mathbf{j}_s^i + cT_s^i(\mathbf{p}) \left[L_s^i(\mathbf{p}) \frac{\sim \mathbf{p}}{|\sim \mathbf{p}|} \cdot \mathbf{j}_s^i - ss' L_{s'}^j(\mathbf{p}') \frac{\mathbf{p}'}{|\mathbf{p}'|} \cdot \mathbf{j}_{s'}^j \right] \\
&= cL_s^i(\mathbf{p}) \left[\frac{\mathbf{p}}{|\mathbf{p}|} - \frac{\sim \mathbf{p}}{|\sim \mathbf{p}|} \right] \cdot \mathbf{j}_s^i + cT_s^i(\mathbf{p}) L_s^i(\mathbf{p}) \left[\frac{\sim \mathbf{p}}{|\sim \mathbf{p}|} \cdot \mathbf{j}_s^i - ss' \frac{c_s^i}{c_{s'}^j} \frac{\mathbf{p}'}{|\mathbf{p}'|} \cdot \mathbf{j}_{s'}^j \right] \\
&= 2cL_s^i(\mathbf{p}) \frac{p_x}{|\mathbf{p}|} j_{s,x}^i + cT_s^i(\mathbf{p}) L_s^i(\mathbf{p}) \left[\frac{\sim \mathbf{p}}{|\sim \mathbf{p}|} \cdot \mathbf{j}_s^i - ss' \frac{c_s^i}{c_{s'}^j} \frac{\mathbf{p}'}{|\mathbf{p}'|} \cdot \mathbf{j}_{s'}^j \right],
\end{aligned}$$

where it was used that $L_{s'}^j(\mathbf{p}') = \frac{c_s^i}{c_{s'}^j} L_s^i(\mathbf{p})$ and $\mathbf{p} - \sim \mathbf{p} = (2p_x, 0)$.

Now we apply the same procedure by multiplying the previous expression for μ and integrating on $\mathbb{R}_{\text{in}}^{2,i}$ obtaining

$$\begin{aligned}
\int_{\mathbb{R}_{\text{in}}^{2,i}} h_s^i(\mathbf{p}) \mu d\mathbf{p} &= 2c \int_{\mathbb{R}_{\text{in}}^{2,i}} L_s^i(\mathbf{p}) \frac{p_x}{|\mathbf{p}|} j_{s,x}^i \mu d\mathbf{p} \\
&+ c \int_{\mathbb{R}_{\text{in}}^{2,i}} T_s^i(\mathbf{p}) L_s^i(\mathbf{p}) \left[\frac{\sim \mathbf{p}}{|\sim \mathbf{p}|} \cdot \mathbf{j}_s^i - ss' \frac{c_s^i}{c_{s'}^j} \frac{\mathbf{p}'}{|\mathbf{p}'|} \cdot \mathbf{j}_{s'}^j \right] \mu d\mathbf{p} \\
&= 2c^2 \int_{\mathbb{R}_{\text{in}}^{2,i}} L_s^i(\mathbf{p}) \left(\frac{p_x}{|\mathbf{p}|} \right)^2 j_{s,x}^i d\mathbf{p} + c^2 \int_{\mathbb{R}_{\text{in}}^{2,i}} T_s^i(\mathbf{p}) L_s^i(\mathbf{p}) \left[\frac{\sim \mathbf{p}}{|\sim \mathbf{p}|} \cdot \mathbf{j}_s^i - ss' \frac{c_s^i}{c_{s'}^j} \frac{\mathbf{p}'}{|\mathbf{p}'|} \cdot \mathbf{j}_{s'}^j \right] \frac{p_x}{|\mathbf{p}|} d\mathbf{p} \\
&= c^2 \int_{\mathbb{R}^2} L_s^i(\mathbf{p}) \left(\frac{p_x}{|\mathbf{p}|} \right)^2 j_{s,x}^i d\mathbf{p} + c^2 \int_{\mathbb{R}_{\text{in}}^{2,i}} T_s^i(\mathbf{p}) L_s^i(\mathbf{p}) \left[\frac{-p_x}{|\mathbf{p}|} j_{s,x}^i - ss' \frac{c_s^i}{c_{s'}^j} \frac{p'_x}{|\mathbf{p}'|} j_{s',x}^j \right] \frac{p_x}{|\mathbf{p}|} d\mathbf{p}
\end{aligned}$$

where in the first term we considered the symmetry with respect to x and in the second one the terms with $p_y j_{s,y}^i$ disappear because of symmetry. By setting

$$H_s^i = \int_{\mathbb{R}_{\text{in}}^{2,i}} h_s^i(\mathbf{p}) \frac{p_x}{|\mathbf{p}|} d\mathbf{p} \quad (5.52)$$

and by splitting different cases we have

$$\begin{aligned} H_+^1 &= c^2 j_{+,x}^1 \int_{\mathbb{R}^2} L_+^1(\mathbf{p}) \left(\frac{p_x}{|\mathbf{p}|} \right)^2 d\mathbf{p} + c^2 j_{+,x}^1 \int_{\{\mathbf{p} \in \mathbb{R}^2 | p_x < 0\}} T_+^1(\mathbf{p}) L_+^1(\mathbf{p}) \left[\frac{-p_x}{|\mathbf{p}|} \right] \frac{p_x}{|\mathbf{p}|} d\mathbf{p} \\ &\quad - c^2 \frac{c_+^1}{c_+^2} j_{+,x}^2 \int_{\{\mathbf{p} \in \mathbb{R}^2 | p_x < 0, c|\mathbf{p}| > \delta V\}} T_+^1(\mathbf{p}) L_+^1(\mathbf{p}) \frac{p'_x}{|\mathbf{p}'|} \frac{p_x}{|\mathbf{p}|} d\mathbf{p} \\ &\quad + c^2 \frac{c_+^1}{c_-^2} j_{-,x}^2 \int_{\{\mathbf{p} \in \mathbb{R}^2 | p_x < 0, c|\mathbf{p}| < \delta V\}} T_+^1(\mathbf{p}) L_+^1(\mathbf{p}) \frac{p'_x}{|\mathbf{p}'|} \frac{p_x}{|\mathbf{p}|} d\mathbf{p} \\ &\quad (i = 1, j = 2, s = +, s' = \pm) \end{aligned}$$

$$\begin{aligned} H_-^1 &= c^2 j_{-,x}^1 \int_{\mathbb{R}^2} L_-^1(\mathbf{p}) \left(\frac{p_x}{|\mathbf{p}|} \right)^2 d\mathbf{p} + c^2 j_{-,x}^1 \int_{\{\mathbf{p} \in \mathbb{R}^2 | p_x < 0\}} T_-^1(\mathbf{p}) L_-^1(\mathbf{p}) \left[\frac{-p_x}{|\mathbf{p}|} \right] \frac{p_x}{|\mathbf{p}|} d\mathbf{p} \\ &\quad - c^2 \frac{c_-^1}{c_-^2} j_{-,x}^2 \int_{\{\mathbf{p} \in \mathbb{R}^2 | p_x < 0\}} T_-^1(\mathbf{p}) L_-^1(\mathbf{p}) \frac{p'_x}{|\mathbf{p}'|} \frac{p_x}{|\mathbf{p}|} d\mathbf{p} \\ &\quad (i = 1, j = 2, s = -, s' = -) \end{aligned}$$

$$\begin{aligned} H_+^2 &= c^2 j_{+,x}^2 \int_{\mathbb{R}^2} L_+^2(\mathbf{p}) \left(\frac{p_x}{|\mathbf{p}|} \right)^2 d\mathbf{p} + c^2 j_{+,x}^2 \int_{\{\mathbf{p} \in \mathbb{R}^2 | p_x > 0\}} T_+^2(\mathbf{p}) L_+^2(\mathbf{p}) \left[\frac{-p_x}{|\mathbf{p}|} \right] \frac{p_x}{|\mathbf{p}|} d\mathbf{p} \\ &\quad - c^2 \frac{c_+^2}{c_+^1} j_{+,x}^1 \int_{\{\mathbf{p} \in \mathbb{R}^2 | p_x > 0\}} T_+^2(\mathbf{p}) L_+^2(\mathbf{p}) \frac{p'_x}{|\mathbf{p}'|} \frac{p_x}{|\mathbf{p}|} d\mathbf{p} \\ &\quad (i = 2, j = 1, s = +, s' = +) \end{aligned}$$

$$\begin{aligned} H_-^2 &= c^2 j_{-,x}^2 \int_{\mathbb{R}^2} L_-^2(\mathbf{p}) \left(\frac{p_x}{|\mathbf{p}|} \right)^2 d\mathbf{p} + c^2 j_{-,x}^2 \int_{\{\mathbf{p} \in \mathbb{R}^2 | p_x > 0\}} T_-^2(\mathbf{p}) L_-^2(\mathbf{p}) \left[\frac{-p_x}{|\mathbf{p}|} \right] \frac{p_x}{|\mathbf{p}|} d\mathbf{p} \\ &\quad + c^2 \frac{c_-^2}{c_+^1} j_{+,x}^1 \int_{\{\mathbf{p} \in \mathbb{R}^2 | p_x > 0, c|\mathbf{p}| > \delta V\}} T_-^2(\mathbf{p}) L_-^2(\mathbf{p}) \frac{p'_x}{|\mathbf{p}'|} \frac{p_x}{|\mathbf{p}|} d\mathbf{p} \\ &\quad - c^2 \frac{c_-^2}{c_-^1} j_{-,x}^1 \int_{\{\mathbf{p} \in \mathbb{R}^2 | p_x > 0, c|\mathbf{p}| < \delta V\}} T_-^2(\mathbf{p}) L_-^2(\mathbf{p}) \frac{p'_x}{|\mathbf{p}'|} \frac{p_x}{|\mathbf{p}|} d\mathbf{p} \\ &\quad (i = 2, j = 1, s = -, s' = \pm) \end{aligned}$$

The next step consists to introduce the Maxwell-Boltzmann approximation, that is

$$c_s^i \approx \frac{n_s^i}{n_0}, \quad L_s^i(\mathbf{p}) \approx M(\mathbf{p}), \quad (5.53)$$

leading to

$$\begin{aligned} H_+^1 &= c^2 j_{+,x}^1 \int_{\mathbb{R}^2} M(\mathbf{p}) \left(\frac{p_x}{|\mathbf{p}|} \right)^2 d\mathbf{p} + c^2 j_{+,x}^1 \int_{\{\mathbf{p} \in \mathbb{R}^2 | p_x < 0\}} T_+^1(\mathbf{p}) M(\mathbf{p}) \left[\frac{-p_x}{|\mathbf{p}|} \right] \frac{p_x}{|\mathbf{p}|} d\mathbf{p} \\ &\quad - c^2 \frac{n_+^1}{n_+^2} j_{+,x}^2 \int_{\{\mathbf{p} \in \mathbb{R}^2 | p_x < 0, c|\mathbf{p}| > \delta V\}} T_+^1(\mathbf{p}) M(\mathbf{p}) \frac{p'_x}{|\mathbf{p}'|} \frac{p_x}{|\mathbf{p}|} d\mathbf{p} \\ &\quad + c^2 \frac{n_+^1}{n_-^2} j_{-,x}^2 \int_{\{\mathbf{p} \in \mathbb{R}^2 | p_x < 0, c|\mathbf{p}| < \delta V\}} T_+^1(\mathbf{p}) M(\mathbf{p}) \frac{p'_x}{|\mathbf{p}'|} \frac{p_x}{|\mathbf{p}|} d\mathbf{p} \\ &\quad (i = 1, j = 2, s = +, s' = \pm) \end{aligned}$$

$$\begin{aligned} H_-^1 &= c^2 j_{-,x}^1 \int_{\mathbb{R}^2} M(\mathbf{p}) \left(\frac{p_x}{|\mathbf{p}|} \right)^2 d\mathbf{p} + c^2 j_{-,x}^1 \int_{\{\mathbf{p} \in \mathbb{R}^2 | p_x < 0\}} T_-^1(\mathbf{p}) M(\mathbf{p}) \left[\frac{-p_x}{|\mathbf{p}|} \right] \frac{p_x}{|\mathbf{p}|} d\mathbf{p} \\ &\quad - c^2 \frac{n_-^1}{n_-^2} j_{-,x}^2 \int_{\{\mathbf{p} \in \mathbb{R}^2 | p_x < 0\}} T_-^1(\mathbf{p}) M(\mathbf{p}) \frac{p'_x}{|\mathbf{p}'|} \frac{p_x}{|\mathbf{p}|} d\mathbf{p} \\ &\quad (i = 1, j = 2, s = -, s' = -) \end{aligned}$$

$$\begin{aligned} H_+^2 &= c^2 j_{+,x}^2 \int_{\mathbb{R}^2} M(\mathbf{p}) \left(\frac{p_x}{|\mathbf{p}|} \right)^2 d\mathbf{p} + c^2 j_{+,x}^2 \int_{\{\mathbf{p} \in \mathbb{R}^2 | p_x > 0\}} T_+^2(\mathbf{p}) M(\mathbf{p}) \left[\frac{-p_x}{|\mathbf{p}|} \right] \frac{p_x}{|\mathbf{p}|} d\mathbf{p} \\ &\quad - c^2 \frac{n_+^2}{n_+^1} j_{+,x}^1 \int_{\{\mathbf{p} \in \mathbb{R}^2 | p_x > 0\}} T_+^2(\mathbf{p}) M(\mathbf{p}) \frac{p'_x}{|\mathbf{p}'|} \frac{p_x}{|\mathbf{p}|} d\mathbf{p} \\ &\quad (i = 2, j = 1, s = +, s' = +) \end{aligned}$$

$$\begin{aligned} H_-^2 &= c^2 j_{-,x}^2 \int_{\mathbb{R}^2} M(\mathbf{p}) \left(\frac{p_x}{|\mathbf{p}|} \right)^2 d\mathbf{p} + c^2 j_{-,x}^2 \int_{\{\mathbf{p} \in \mathbb{R}^2 | p_x > 0\}} T_-^2(\mathbf{p}) M(\mathbf{p}) \left[\frac{-p_x}{|\mathbf{p}|} \right] \frac{p_x}{|\mathbf{p}|} d\mathbf{p} \\ &\quad + c^2 \frac{n_-^2}{n_+^1} j_{+,x}^1 \int_{\{\mathbf{p} \in \mathbb{R}^2 | p_x > 0, c|\mathbf{p}| > \delta V\}} T_-^2(\mathbf{p}) M(\mathbf{p}) \frac{p'_x}{|\mathbf{p}'|} \frac{p_x}{|\mathbf{p}|} d\mathbf{p} \\ &\quad - c^2 \frac{n_-^2}{n_-^1} j_{-,x}^1 \int_{\{\mathbf{p} \in \mathbb{R}^2 | p_x > 0, c|\mathbf{p}| < \delta V\}} T_-^2(\mathbf{p}) M(\mathbf{p}) \frac{p'_x}{|\mathbf{p}'|} \frac{p_x}{|\mathbf{p}|} d\mathbf{p} \\ &\quad (i = 2, j = 1, s = -, s' = \pm). \end{aligned}$$

Now we compute the integral

$$\int_{\mathbb{R}^2} M(\mathbf{p}) \left(\frac{p_x}{|\mathbf{p}|} \right)^2 d\mathbf{p} = \int_{\mathbb{R}^2} \frac{e^{-\beta c |\mathbf{p}|}}{n_0} \left(\frac{p_x}{|\mathbf{p}|} \right)^2 d\mathbf{p}. \quad (5.54)$$

Then by performing the change of variables

$$\begin{cases} p_x = \rho \cos \vartheta \\ p_y = \rho \sin \vartheta \end{cases} \quad (5.55)$$

where $\rho = |\mathbf{p}|$ it becomes

$$\int_0^{2\pi} d\vartheta \int_0^{+\infty} \frac{e^{-\beta c \rho}}{n_0} \frac{\rho^2 \cos^2 \vartheta}{\rho^2} \rho d\rho = \int_0^{2\pi} \cos^2 \vartheta d\vartheta \int_0^{+\infty} \frac{e^{-\beta c \rho}}{n_0} \rho d\rho \quad (5.56)$$

and by setting $\beta c \rho = t$ we have

$$\int_0^{2\pi} \cos^2 \vartheta d\vartheta \int_0^{+\infty} \frac{e^{-\beta c \rho}}{n_0} \rho d\rho = \frac{1}{n_0 (\beta c)^2} \int_0^{2\pi} \cos^2 \vartheta d\vartheta \int_0^{+\infty} e^{-t} t dt = \frac{\pi}{n_0 (\beta c)^2} = \frac{h^2}{2}. \quad (5.57)$$

In this way the source terms write

$$\begin{aligned} H_+^1 &= c^2 j_{+,x}^1 \frac{h^2}{2} + c^2 j_{+,x}^1 \int_{\{\mathbf{p} \in \mathbb{R}^2 | p_x < 0\}} T_+^1(\mathbf{p}) M(\mathbf{p}) \left[\frac{-p_x}{|\mathbf{p}|} \right] \frac{p_x}{|\mathbf{p}|} d\mathbf{p} \\ &\quad - c^2 \frac{n_+^1}{n_+^2} j_{+,x}^2 \int_{\{\mathbf{p} \in \mathbb{R}^2 | p_x < 0, c|\mathbf{p}| > \delta V\}} T_+^1(\mathbf{p}) M(\mathbf{p}) \frac{p'_x}{|\mathbf{p}'|} \frac{p_x}{|\mathbf{p}|} d\mathbf{p} \\ &\quad + c^2 \frac{n_+^1}{n_-^2} j_{-,x}^2 \int_{\{\mathbf{p} \in \mathbb{R}^2 | p_x < 0, c|\mathbf{p}| < \delta V\}} T_+^1(\mathbf{p}) M(\mathbf{p}) \frac{p'_x}{|\mathbf{p}'|} \frac{p_x}{|\mathbf{p}|} d\mathbf{p} \\ &\quad (i = 1, j = 2, s = +, s' = \pm) \end{aligned}$$

$$\begin{aligned} H_-^1 &= c^2 j_{-,x}^1 \frac{h^2}{2} + c^2 j_{-,x}^1 \int_{\{\mathbf{p} \in \mathbb{R}^2 | p_x < 0\}} T_-^1(\mathbf{p}) M(\mathbf{p}) \left[\frac{-p_x}{|\mathbf{p}|} \right] \frac{p_x}{|\mathbf{p}|} d\mathbf{p} \\ &\quad - c^2 \frac{n_-^1}{n_-^2} j_{-,x}^2 \int_{\{\mathbf{p} \in \mathbb{R}^2 | p_x < 0\}} T_-^1(\mathbf{p}) M(\mathbf{p}) \frac{p'_x}{|\mathbf{p}'|} \frac{p_x}{|\mathbf{p}|} d\mathbf{p} \\ &\quad (i = 1, j = 2, s = -, s' = -) \end{aligned}$$

$$\begin{aligned}
H_+^2 &= c^2 j_{+,x}^2 \frac{h^2}{2} + c^2 j_{+,x}^2 \int_{\{\mathbf{p} \in \mathbb{R}^2 | p_x > 0\}} T_+^2(\mathbf{p}) M(\mathbf{p}) \left[\frac{-p_x}{|\mathbf{p}|} \right] \frac{p_x}{|\mathbf{p}|} d\mathbf{p} \\
&\quad - c^2 \frac{n_+^2}{n_+^1} j_{+,x}^1 \int_{\{\mathbf{p} \in \mathbb{R}^2 | p_x > 0\}} T_+^2(\mathbf{p}) M(\mathbf{p}) \frac{p'_x}{|\mathbf{p}'|} \frac{p_x}{|\mathbf{p}|} d\mathbf{p} \\
&\quad (i = 2, j = 1, s = +, s' = +)
\end{aligned}$$

$$\begin{aligned}
H_-^2 &= c^2 j_{-,x}^2 \frac{h^2}{2} + c^2 j_{-,x}^2 \int_{\{\mathbf{p} \in \mathbb{R}^2 | p_x > 0\}} T_-^2(\mathbf{p}) M(\mathbf{p}) \left[\frac{-p_x}{|\mathbf{p}|} \right] \frac{p_x}{|\mathbf{p}|} d\mathbf{p} \\
&\quad + c^2 \frac{n_-^2}{n_-^1} j_{+,x}^1 \int_{\{\mathbf{p} \in \mathbb{R}^2 | p_x > 0, c|\mathbf{p}| > \delta V\}} T_-^2(\mathbf{p}) M(\mathbf{p}) \frac{p'_x}{|\mathbf{p}'|} \frac{p_x}{|\mathbf{p}|} d\mathbf{p} \\
&\quad - c^2 \frac{n_-^2}{n_-^1} j_{-,x}^1 \int_{\{\mathbf{p} \in \mathbb{R}^2 | p_x > 0, c|\mathbf{p}| < \delta V\}} T_-^2(\mathbf{p}) M(\mathbf{p}) \frac{p'_x}{|\mathbf{p}'|} \frac{p_x}{|\mathbf{p}|} d\mathbf{p} \\
&\quad (i = 2, j = 1, s = -, s' = \pm).
\end{aligned}$$

Finally by imposing the interface conditions and computing $p'_x/|\mathbf{p}'|$ as

$$\nu_{\pm}(\mathbf{p}) = \frac{\sqrt{|c|\mathbf{p}| \pm \delta V|^2 - c^2 p_y^2}}{|c|\mathbf{p}| \pm \delta V|} \quad (5.58)$$

we have

$$\begin{aligned}
H_+^1 &= c^2 j_{+,x}^1 \frac{h^2}{2} + c^2 j_{+,x}^1 \int_{\{\mathbf{p} \in \mathbb{R}^2 | p_x < 0\}} T_+^1(\mathbf{p}) M(\mathbf{p}) \left[\frac{-p_x}{|\mathbf{p}|} \right] \frac{p_x}{|\mathbf{p}|} d\mathbf{p} \\
&\quad - c^2 \frac{n_+^1}{n_+^2} j_{+,x}^2 \int_{\{\mathbf{p} \in \mathbb{R}^2 | p_x < 0, c|\mathbf{p}| > \delta V\}} T_+^1(\mathbf{p}) M(\mathbf{p}) \nu_-(\mathbf{p}) \frac{p_x}{|\mathbf{p}|} d\mathbf{p} \\
&\quad + c^2 \frac{n_+^1}{n_+^2} j_{-,x}^2 \int_{\{\mathbf{p} \in \mathbb{R}^2 | p_x < 0, c|\mathbf{p}| < \delta V\}} T_+^1(\mathbf{p}) M(\mathbf{p}) \nu_-(\mathbf{p}) \frac{p_x}{|\mathbf{p}|} d\mathbf{p} \\
&\quad (i = 1, j = 2, s = +, s' = \pm)
\end{aligned}$$

$$\begin{aligned}
H_-^1 &= c^2 j_{-,x}^1 \frac{h^2}{2} + c^2 j_{-,x}^1 \int_{\{\mathbf{p} \in \mathbb{R}^2 | p_x < 0\}} T_-^1(\mathbf{p}) M(\mathbf{p}) \left[\frac{-p_x}{|\mathbf{p}|} \right] \frac{p_x}{|\mathbf{p}|} d\mathbf{p} \\
&\quad - c^2 \frac{n_-^1}{n_-^2} j_{-,x}^2 \int_{\{\mathbf{p} \in \mathbb{R}^2 | p_x < 0\}} T_-^1(\mathbf{p}) M(\mathbf{p}) \nu_+(\mathbf{p}) \frac{p_x}{|\mathbf{p}|} d\mathbf{p} \\
&\quad (i = 1, j = 2, s = -, s' = -)
\end{aligned}$$

$$\begin{aligned}
H_+^2 &= c^2 j_{+,x}^2 \frac{h^2}{2} + c^2 j_{+,x}^2 \int_{\{\mathbf{p} \in \mathbb{R}^2 | p_x > 0\}} T_+^2(\mathbf{p}) M(\mathbf{p}) \left[\frac{-p_x}{|\mathbf{p}|} \right] \frac{p_x}{|\mathbf{p}|} d\mathbf{p} \\
&\quad - c^2 \frac{n_+^2}{n_+^1} j_{+,x}^1 \int_{\{\mathbf{p} \in \mathbb{R}^2 | p_x > 0\}} T_+^2(\mathbf{p}) M(\mathbf{p}) \nu_+(\mathbf{p}) \frac{p_x}{|\mathbf{p}|} d\mathbf{p} \\
&\quad (i = 2, j = 1, s = +, s' = +)
\end{aligned}$$

$$\begin{aligned}
H_-^2 &= c^2 j_{-,x}^2 \frac{h^2}{2} + c^2 j_{-,x}^2 \int_{\{\mathbf{p} \in \mathbb{R}^2 | p_x > 0\}} T_-^2(\mathbf{p}) M(\mathbf{p}) \left[\frac{-p_x}{|\mathbf{p}|} \right] \frac{p_x}{|\mathbf{p}|} d\mathbf{p} \\
&\quad + c^2 \frac{n_-^2}{n_+^1} j_{+,x}^1 \int_{\{\mathbf{p} \in \mathbb{R}^2 | p_x > 0, c|\mathbf{p}| > \delta V\}} T_-^2(\mathbf{p}) M(\mathbf{p}) \nu_-(\mathbf{p}) \frac{p_x}{|\mathbf{p}|} d\mathbf{p} \\
&\quad - c^2 \frac{n_-^2}{n_-^1} j_{-,x}^1 \int_{\{\mathbf{p} \in \mathbb{R}^2 | p_x > 0, c|\mathbf{p}| < \delta V\}} T_-^2(\mathbf{p}) M(\mathbf{p}) \nu_-(\mathbf{p}) \frac{p_x}{|\mathbf{p}|} d\mathbf{p} \\
&\quad (i = 2, j = 1, s = -, s' = \pm).
\end{aligned}$$

5.1.3 Approximation of interface conditions

The quantities n_s^i / n_s^j can be approximated as follows:

$$\frac{n_+^1}{n_+^2} = \frac{e^{\beta\delta V} n_+^2 + O(\tau)}{n_+^2} = e^{\beta\delta V} (1 + O(\tau)) = e^{\beta\delta V} + O(\tau), \quad (5.59)$$

$$\frac{n_+^2}{n_+^1} = \frac{n_+^2}{e^{\beta\delta V} n_+^2 + O(\tau)} = e^{-\beta\delta V} \frac{1}{1 + O(\tau)} \approx e^{-\beta\delta V} + O(\tau), \quad (5.60)$$

$$\frac{n_-^1}{n_-^2} = \frac{e^{-\beta\delta V} n_-^2 + O(\tau)}{n_-^2} = e^{-\beta\delta V} (1 + O(\tau)) = e^{-\beta\delta V} + O(\tau), \quad (5.61)$$

$$\frac{n_-^2}{n_-^1} = \frac{n_-^2}{e^{-\beta\delta V} n_-^2 + O(\tau)} = e^{\beta\delta V} \frac{1}{1 + O(\tau)} \approx e^{\beta\delta V} + O(\tau). \quad (5.62)$$

By using the previous relations and by canceling a factor c appearing in all quantities A, B, C, D and H_s^i we obtain the final expressions

$$\begin{aligned}
A &= - \int_{\{\mathbf{p} \in \mathbb{R}^2 | p_x > 0, c|\mathbf{p}| > \delta V\}} T_+^1(\mathbf{p}) M(\mathbf{p}) \frac{p_x}{|\mathbf{p}|} d\mathbf{p} \\
B &= - \frac{n_0}{n_-^2} \int_{\{\mathbf{p} \in \mathbb{R}^2 | p_x > 0, c|\mathbf{p}| < \delta V\}} T_+^1(\mathbf{p}) M(\mathbf{p}) \frac{p_x}{|\mathbf{p}|} d\mathbf{p} \\
C &= - \int_{\{\mathbf{p} \in \mathbb{R}^2 | p_x > 0\}} T_-^1(\mathbf{p}) M(\mathbf{p}) \frac{p_x}{|\mathbf{p}|} d\mathbf{p} \\
D &= e^{-\beta\delta V} \int_{\{\mathbf{p} \in \mathbb{R}^2 | p_x > 0\}} T_+^2(\mathbf{p}) M(\mathbf{p}) \frac{p_x}{|\mathbf{p}|} d\mathbf{p}
\end{aligned}$$

$$\begin{aligned}
H_+^1 &= c j_{+,x}^1 \frac{h^2}{2} + c j_{+,x}^1 \int_{\{\mathbf{p} \in \mathbb{R}^2 | p_x < 0\}} T_+^1(\mathbf{p}) M(\mathbf{p}) \left[\frac{-p_x}{|\mathbf{p}|} \right] \frac{p_x}{|\mathbf{p}|} d\mathbf{p} \\
&\quad - c e^{\beta \delta V} j_{+,x}^2 \int_{\{\mathbf{p} \in \mathbb{R}^2 | p_x < 0, c|\mathbf{p}| > \delta V\}} T_+^1(\mathbf{p}) M(\mathbf{p}) \nu_-(\mathbf{p}) \frac{p_x}{|\mathbf{p}|} d\mathbf{p} \\
&\quad + c \frac{n_+^1}{n_-^2} j_{-,x}^2 \int_{\{\mathbf{p} \in \mathbb{R}^2 | p_x < 0, c|\mathbf{p}| < \delta V\}} T_+^1(\mathbf{p}) M(\mathbf{p}) \nu_-(\mathbf{p}) \frac{p_x}{|\mathbf{p}|} d\mathbf{p} \\
&\quad (i = 1, j = 2, s = +, s' = \pm)
\end{aligned}$$

$$\begin{aligned}
H_-^1 &= c j_{-,x}^1 \frac{h^2}{2} + c j_{-,x}^1 \int_{\{\mathbf{p} \in \mathbb{R}^2 | p_x < 0\}} T_-^1(\mathbf{p}) M(\mathbf{p}) \left[\frac{-p_x}{|\mathbf{p}|} \right] \frac{p_x}{|\mathbf{p}|} d\mathbf{p} \\
&\quad - c e^{-\beta \delta V} j_{-,x}^2 \int_{\{\mathbf{p} \in \mathbb{R}^2 | p_x < 0\}} T_-^1(\mathbf{p}) M(\mathbf{p}) \nu_+(\mathbf{p}) \frac{p_x}{|\mathbf{p}|} d\mathbf{p} \\
&\quad (i = 1, j = 2, s = -, s' = -)
\end{aligned}$$

$$\begin{aligned}
H_+^2 &= c j_{+,x}^2 \frac{h^2}{2} + c j_{+,x}^2 \int_{\{\mathbf{p} \in \mathbb{R}^2 | p_x > 0\}} T_+^2(\mathbf{p}) M(\mathbf{p}) \left[\frac{-p_x}{|\mathbf{p}|} \right] \frac{p_x}{|\mathbf{p}|} d\mathbf{p} \\
&\quad - c e^{-\beta \delta V} j_{+,x}^1 \int_{\{\mathbf{p} \in \mathbb{R}^2 | p_x > 0\}} T_+^2(\mathbf{p}) M(\mathbf{p}) \nu_+(\mathbf{p}) \frac{p_x}{|\mathbf{p}|} d\mathbf{p} \\
&\quad (i = 2, j = 1, s = +, s' = +)
\end{aligned}$$

$$\begin{aligned}
H_-^2 &= c j_{-,x}^2 \frac{h^2}{2} + c j_{-,x}^2 \int_{\{\mathbf{p} \in \mathbb{R}^2 | p_x > 0\}} T_-^2(\mathbf{p}) M(\mathbf{p}) \left[\frac{-p_x}{|\mathbf{p}|} \right] \frac{p_x}{|\mathbf{p}|} d\mathbf{p} \\
&\quad + c \frac{n_-^2}{n_+^1} j_{+,x}^1 \int_{\{\mathbf{p} \in \mathbb{R}^2 | p_x > 0, c|\mathbf{p}| > \delta V\}} T_-^2(\mathbf{p}) M(\mathbf{p}) \nu_-(\mathbf{p}) \frac{p_x}{|\mathbf{p}|} d\mathbf{p} \\
&\quad - c e^{-\beta \delta V} j_{-,x}^1 \int_{\{\mathbf{p} \in \mathbb{R}^2 | p_x > 0, c|\mathbf{p}| < \delta V\}} T_-^2(\mathbf{p}) M(\mathbf{p}) \nu_-(\mathbf{p}) \frac{p_x}{|\mathbf{p}|} d\mathbf{p} \\
&\quad (i = 2, j = 1, s = -, s' = \pm),
\end{aligned}$$

where

$$\nu_{\pm}(\mathbf{p}) = \frac{\sqrt{|c|\mathbf{p}| \pm \delta V|^2 - c^2 p_y^2}}{|c|\mathbf{p}| \pm \delta V|} \quad (5.63)$$

and the quantities written above are related to the corrections at first order in τ through

$$\begin{cases} \rho_+^1 - \frac{n_+^1}{n_+^2} \rho_+^2 = -\frac{H_+^2}{D} \\ \rho_-^1 - \frac{n_-^1}{n_-^2} \rho_-^2 = \frac{H_-^1}{C} \\ \frac{n_-^2 \rho_+^1 + n_+^1 \rho_-^2}{n_0} = \frac{H_+^1}{B} + \frac{A H_+^2}{DB} \end{cases} \quad (5.64)$$

5.1.4 Evaluation of the asymptotic densities for electrons

Solving the Milne problem (5.5)-(5.7) in order to obtain the asymptotic densities $n_s^{i,\infty}$ implies that a “kinetic” stage is still needed in our diffusive model. This is not very appealing, when looking for a simple and numerically light model. Then, we should resort to some kind of approximation of the Milne problem [32, 39].

The simplest possible approach is the already mentioned Marshack approximation, which amounts to assuming that the solution of (5.5) has approximately the asymptotic form

$$f_s^i \approx L_s^i n_s^{i,\infty},$$

so that the parameters $n_s^{i,\infty}$ are simply obtained by imposing the conditions (5.7).

Let us consider the case $\delta V = 0$, which is our case of interest [108]. Then, the DTC for electrons and holes get decoupled and the DTC (5.12) reduce to

$$A(n_s^1) - A(n_s^2) = \frac{\tau}{n_0} \left(\frac{n_s^{2,\infty}}{c_s^2} - \frac{n_s^{1,\infty}}{c_s^1} \right), \quad (5.65)$$

and we recall that the conservation of the x -flow through the interface holds separately for electrons and holes:

$$j_{s,x}^1 = j_{s,x}^2 = j_{s,x}, \quad s = \pm 1$$

(here, $j_{s,x}$ is intended to be evaluated at the interface $x = 0$). Focusing on electrons ($s = +1$) it turns out that, in the Marshack approximation,

$$A(n_+^1) - A(n_+^2) = \frac{\tau}{n_0} \left(\frac{n_+^{2,\infty}}{c_+^2} - \frac{n_+^{1,\infty}}{c_+^1} \right) = \tau j_{+,x} q_+ \quad (5.66)$$

where

$$q_+ = \frac{v_F}{n_0} \frac{\int L_+^2 \mu^2 d\mathbf{p} - 2 \int_{p_x > 0} T_+^1 L_+^2 \mu^2 d\mathbf{p}}{c_+^2 \int_{p_x > 0} T_+^1 L_+^2 \mu d\mathbf{p}}. \quad (5.67)$$

and we have put

$$\mu = \mu(\mathbf{p}) := \frac{p_x}{|\mathbf{p}|}.$$

Note that q_+ (which may depend on y) is the equivalent of the interpolation constant of Ref. [32] which in turn, is the analogous of the extrapolation constant of neutron transport [5].

In the Maxwell-Boltzmann case the above formulas reduce to the following:

$$n_+^1 - n_+^2 = \tau \left(n_+^{2,\infty} - n_+^{1,\infty} \right) = \tau j_{+,x} q_+, \quad (5.68)$$

$$q_+ = v_F \frac{\frac{h^2}{2} - 2 \int_{p_x > 0} T_+^1 M \mu^2 d\mathbf{p}}{\int_{p_x > 0} T_+^1 M \mu d\mathbf{p}}, \quad (5.69)$$

where h is the Planck constant and M is the Maxwellian (5.11).

We remark that in the y -homogeneous case, the DD equations are 1-dimensional and the currents $j_{s,x}$, $s = \pm 1$, are (separately) constant throughout the device.

5.2 Device modelling

In this section we would like to adopt the model described above for illustrating a more physical situation. In [108] the authors experimentally demonstrated the Klein tunneling effects in graphene. They proposed a device is a graphene heterojunction composed by a back gate, a SiO_2 substrate where the graphene layer is placed on, a layer of HfO_2 , a thin top gate and two metallic source and drain contacts. The situation is depicted in Fig. 5.1. We summarize the model in the case suitable for our application,

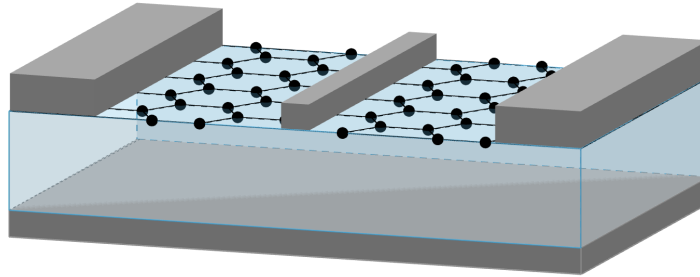


FIGURE 5.1: Schematic representation of a typical graphene heterojunction device.

i.e. $\delta V = 0$ and 1-dimensional (y -homogeneous). Following [108], the form of the potential barrier is determined by two parameter, the top gate voltage V_{tg} and the back

gate voltage V_{bg} . The top gate is strip-shaped, which determines the barrier width D (approximately independent on the value V_{tg}). The barrier height is then given by

$$V_h = V_{tg} - V_{bg},$$

while V_{bg} is the potential outside the barrier and determines the equilibrium carrier concentrations [35].

For the transmission coefficient of a sharp potential barrier let us consider the model proposed in [19]

$$T(\varphi) = \begin{cases} \frac{\cos^2 \theta \cos^2 \varphi}{[\cos(D\sqrt{K}) \cos \varphi \cos \theta]^2 + \sin^2(D\sqrt{K})(1 - ss' \sin \varphi \sin \theta)^2}, & \text{if } K > 0 \\ 0 & \text{if } K < 0 \end{cases} \quad (5.70)$$

where

$$\mathbf{p} = |\mathbf{p}|(\cos(\varphi), \sin(\varphi)), \quad (5.71)$$

$$\theta = \arctan\left(\frac{p_y}{\hbar\sqrt{K}}\right), \quad (5.72)$$

$$s = \text{sgn}(v_F|\mathbf{p}|), \quad s' = \text{sgn}(v_F|\mathbf{p}| - V_h), \quad (5.73)$$

$$K = \left(\frac{v_F|\mathbf{p}| - V_h}{\hbar v_F}\right)^2 - \left(\frac{|\mathbf{p}| \sin(\varphi)}{\hbar}\right)^2. \quad (5.74)$$

The parameter D indicates the barrier width. According to [51], an approximation for high values of the barrier is therefore given by

$$T = \begin{cases} \frac{\cos^2(\varphi)}{1 - \cos^2(D\sqrt{K}) \sin^2(\varphi)}, & \text{if } K > 0, \\ 0, & \text{if } K < 0. \end{cases} \quad (5.75)$$

The model to be solved numerically is therefore structured as follows. Since we focus on electrons, the subscript $+$ is dropped everywhere.

1. The 1-dimensional stationary DD equation

$$\partial_x j = 0, \quad j = -\frac{\tau v_F^2}{2} [\partial_x n + \beta n_0 \phi_1(A(n)) \nabla U],$$

holds separately in the space intervals $(-L, 0)$ and $(0, L)$.

2. The smooth potential $U(x)$ can be considered to be linear, representing an applied voltage (external bias). In a more refined model, U could be self-consistently related

to the density n_+ through the Poisson equation (in this case the bias is imposed as boundary conditions for the Poisson equation).

3. At $x = 0$ we impose the interface conditions

$$\begin{cases} j^1 = j^2 \quad (:= j) \\ A(n^1) - A(n^2) = \tau j q, \end{cases}$$

where, as usual, the upper index denotes the left/right values at $x = 0$, and where $q \equiv q_+$ is given by (5.67) and (5.75).

4. At $x = \pm L$ standard nonhomogeneous Dirichlet conditions are imposed (i.e. we assign the value of $n(L)$ and $n(-L)$).

In the Maxwell Boltzmann approximation, the DD equation reduces to

$$\partial_x j = 0, \quad j = -\frac{\tau v_F^2}{2} [\partial_x n + \beta n \nabla U],$$

and the interface conditions become

$$\begin{cases} j^1 = j^2 \quad (:= j) \\ n^1 - n^2 = \tau j q, \end{cases}$$

where now the interpolation constant is given by (5.69).

A last possible approach is to use the chemical potential A as unknown, instead of the density. In this case the DD equation to be solved is

$$\partial_x j = 0, \quad j = -\frac{\tau v_F^2 n_0}{2} [\partial_x \phi_2(A) + \beta \phi_1(A) \nabla U],$$

that can also be written as

$$\partial_x j = 0, \quad j = -\frac{\tau v_F^2 n_0}{2} \phi_1(A) [\partial_x A + \beta \nabla U],$$

(since $\phi'_k = \phi_{k-1}$). The interface conditions are

$$\begin{cases} j^1 = j^2 \quad (:= j) \\ A^1 - A^2 = \tau j q, \end{cases}$$

(where A^1 and A^2 denote the left and right limit at $x = 0$ of the electron chemical potential) and q is still given by (5.67) and (5.75) but now

$$L^i(\mathbf{p}) := \frac{1}{n_0 \phi_1(A^i)} \frac{e^{\beta v_F |\mathbf{p}| - A^i}}{(e^{\beta v_F |\mathbf{p}| - A^i} + 1)^2}.$$

depends on A^i and not $A(n^i)$ (remember that here $s = +1$ everywhere and so we omitted the index s).

Of course, the values of A at $x = \pm L$ must be specified instead of the values of n .

5.2.1 Numerical method

In the Maxwell-Boltzmann approximation, let us consider the DD equation

$$\partial_x j = 0, \quad j = -\frac{\tau v_F^2}{2} [\partial_x n + \beta n \partial_x U] \quad (5.76)$$

with the interface conditions

$$\begin{cases} j^1 = j^2 \\ n^1 - n^2 = \tau j q \end{cases} \quad (5.77)$$

Now we apply the derivative with respect to x to the current expression getting

$$\partial_{xx} n + \beta \partial_x n \partial_x U = 0 \quad (5.78)$$

If we choose to decompose the domains Ω^1 and Ω^2 in N_x cells with Δx spatial step in x direction by taking index i varying in x direction we obtain the following system of linear equations

$$\frac{n^{i-1} - 2n^i + n^{i+1}}{\Delta x^2} + \beta \partial_x U \frac{n^{i+1} - n^{i-1}}{2\Delta x} = 0, \quad (5.79)$$

with $i = 2, \dots, N_x - 1$, and $i = N_x + 1, \dots, 2N_x - 1$. At $x = \pm L$ we impose Dirichlet boundary conditions

$$n^1 = n^{-L}, \quad n^{2N_x} = n^L. \quad (5.80)$$

At the interface $x = 0$ we need to include relations (5.77). By approximating

$$j^2 \approx \frac{-3n^{N_x+1} + 4n^{N_x+2} - n^{N_x+3}}{2\Delta x} + \beta \partial_x U n^{N_x+1} \quad (5.81)$$

with forward second order finite differences, the second relation becomes

$$n^{N_x} - n^{N_x+1} - \tau q \left[\frac{-3n^{N_x+1} + 4n^{N_x+2} - n^{N_x+3}}{2\Delta x} + \beta \partial_x U n^{N_x+1} \right] = 0 \quad (5.82)$$

and, by approximating

$$j^1 \approx \frac{n^{N_x-2} - 4n^{N_x-1} + 3n^{N_x}}{2\Delta x} + \beta \partial_x U n^{N_x} \quad (5.83)$$

and

$$j^2 \approx \frac{-3n^{N_x+1} + 4n^{N_x+2} - n^{N_x+3}}{2\Delta x} + \beta \partial_x U n^{N_x+1} \quad (5.84)$$

by means of backward and forward second order finite differences respectively we get

$$\frac{n^{N_x-2} - 4n^{N_x-1} + 3n^{N_x}}{2\Delta x} + \beta \partial_x U n^{N_x} - \frac{-3n^{N_x+1} + 4n^{N_x+2} - n^{N_x+3}}{2\Delta x} - \beta \partial_x U n^{N_x+1} = 0 \quad (5.85)$$

Moreover we need to calculate the coefficient q , that is

$$q = v_F \frac{\frac{\hbar^2}{2} - 2 \int_{p_x > 0} T M \mu^2 d\mathbf{p}}{\int_{p_x > 0} T M \mu d\mathbf{p}}. \quad (5.86)$$

For the transmission coefficient, in our simulations we adopt the expression (5.70). We remark that the integration domain is

$$\mathcal{B} = \left\{ \mathbf{p} \in \mathbb{R}^2 \mid p_x > 0 \right\}$$

Since $M(\mathbf{p}) \rightarrow 0$ when $|\mathbf{p}| \rightarrow +\infty$ we can define

$$p_{x,max}, \quad p_{y,max}, \quad p_{max} = \sqrt{p_{x,max}^2 + p_{y,max}^2}.$$

In order to evaluate the coefficients numerically we can approximate

$$\mathcal{B} \approx [0, p_{x,max}] \times [-p_{y,max}, p_{y,max}]$$

and we discretize the domain in $N \times M$ cells, indicate with p_{ij} the center of the (i, j) cell and set $\Delta x = p_{x,max}/N$, $\Delta y = 2p_{y,max}/M$. Finally we obtain

$$\int_{\mathcal{B}} g(\mathbf{p}) d\mathbf{p} \approx \Delta x \Delta y \sum_{i=1}^N \sum_{j=1}^M g(p_{ij}),$$

being g the function to be integrated.

5.2.2 Numerical results

In this section we show some numerical simulation regarding the model described above. In order to get the charge density at contacts we remark that in graphene it is

related to the applied voltage and consists of the sum of a work function, due to the metal-graphene contact, that shifts the potential at contacts by V_{wf} , and a bias applied in one of the contacts,

$$V_S = V_{wf}, \quad V_D = V_{wf} + V_{bias}. \quad (5.87)$$

Following [53], the electron densities are given by

$$n^{-L} = \phi_1(qV_S), \quad n^L = \phi_1(qV_D). \quad (5.88)$$

In [108] is presented a device in which a quantum barrier is obtained by applying a thin metallic gate on the graphene layer of gate voltage V_{TG} . Moreover a back gate of the dimensions of all the device of voltage V_{BG} determines the doping. The reason is the property of quantum capacitance of graphene (see [108, 53]). The effect due to the gate is related to the distance between the gate and the graphene layer and also to the materials adopted as substrates. They present also a reduced mode to quantify the effect under consideration. To have more physically accurate simulation we need to couple the above presented model with a Poisson equation solved in the device domain. Here some preliminary numerical results are obtained by modulating the top gate voltage with a tuning parameter in order to reproduce a reasonable value of the voltage applied on the graphene layer, that is $V_h = cV_{TG}$, being c a constant. Similarly, for the back gate we have adopted $V_b = dV_{BG}$, being d a constant. In our simulations we have chosen $d = 12.8$, according to [108]. Moreover the electric field is approximate to $V_{bias}/2L$, neglecting the effect due to the small gate.

In Figure 5.2 we show the numerical results reproducing the conductance versus the top gate voltage, obtained at different values of $V_{BG} = 0, 0.5$ and 1 V. The value of the work function is $V_{wf} = 0.25$ V and the bias is $V_{bias} = 0.001$. The device total length is $2L = 8 \mu\text{m}$, the width is $W = 1 \mu\text{m}$, the barrier length is 50 nm , the temperature is $T = 40 \text{ K}$, $\tau = 0.1 \text{ ps}$ and $c = 0.05$. As in [108], Fig. 1c, we observe the presence of oscillations in the conductance and the behavior in terms of period looks similar while the conductance values differ for a constant factor (we remark that our simulations refer to the top left area of the plot, due to a different sign convention). In our simulations for low values of the top gate voltage the conductance steeply increase but, at variance with experiments of [108], it does not saturate near the zero value. We hypothesize that this effect is not accurately described because a different model of barrier is needed, e.g., a gradual ascent instead of a sharp one. We remark that the barrier model is determinant in the calculation of the transmission coefficient. On the contrary a correct prediction of the values of conductance requires an inclusion of a more physical mobility model (see [62, 81]) and an accurate determination of the electric field by a Poisson equation (see [82, 79]). A more detailed analysis will be

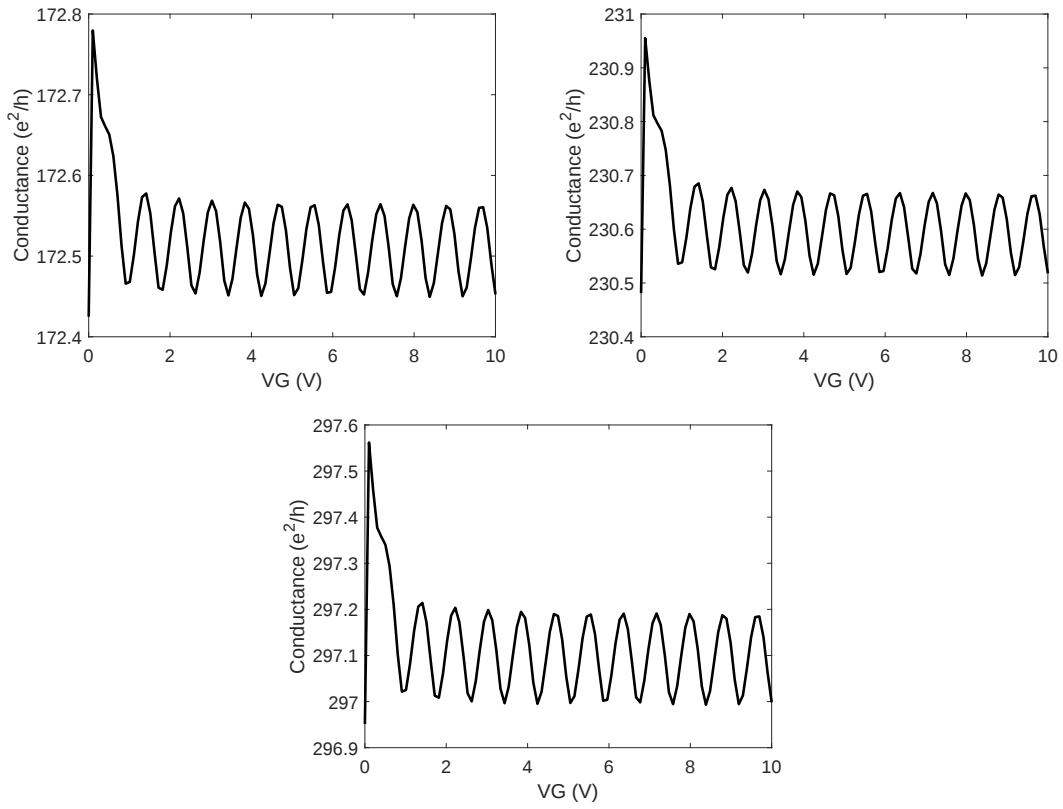


FIGURE 5.2: Conductance versus top gate voltage at $V_{BG} = 0$ V (top-left), 0.5 V (top-right) and 1 V (bottom).

performed together with a complete model implementation. In conclusion the quantum drift diffusion model proposed in this chapter appears to be able to reproduce the Klein tunneling effect in the above described situation.

Chapter 6

Optimal control theory of charge transport in graphene

Nowadays optimization with partial differential equation is a very important research field in applied mathematics for its applications in engineering, industry and social sciences. The purpose of PDE optimization consists to decide how to optimally change features of systems modeled by PDEs. A typical optimal control problem consists of an evolutionary or equilibrium system including a control mechanism and of a functional modeling the purpose of the control. These problems are usually solved considering a Lagrange framework that exploits first-order optimality conditions that are formulated in terms of the governing model, its adjoint counterpart, and a gradient equation (or inequality). Other important classes of optimization problems are shape design, topology, and parameter optimization. For further information about optimal control problems see [15].

In this chapter we explore the possibility to define and numerically solve an optimal control problem involving the semiclassical Boltzmann equation for charge transport in graphene. Numerical approaches based on the Direct Simulation Monte Carlo (DSMC) and on the Discontinuous Galerkin (DG) methods have been formulated, for example, in [89, 25, 24, 63]. An optimal control problem for the Keilson-Storer master equation has been formulated in and solved by means of the DSMC method in [11].

We propose to control the electric field acting on a graphene device in order to force the electrons to obey a target distribution.

The preliminary results included here and the study presented in Ref. [11] have been obtained during a visiting period at the Institut für Mathematik, Julius-Maximilians Universität Würzburg, under the supervision of Prof. A. Borzì.

6.1 Model description

Let us consider the semiclassical Boltzmann equation for electrons belonging to the conduction band in the homogeneous case

$$\frac{\partial f(t, \mathbf{k})}{\partial t} + \mathbf{u}(t) \cdot \nabla_{\mathbf{k}} f(t, \mathbf{k}) = \mathcal{C}[f, f](t, \mathbf{k}),$$

being $f(t, \mathbf{k})$ the distribution function of electrons at time t and wave-vector $\mathbf{k}$, $\mathbf{u}(t)$ a time depending function, related to an external electric field $\mathbf{E}(t)$ by

$$\mathbf{u}(t) = -\frac{e}{\hbar} \mathbf{E}(t), \quad (6.1)$$

playing the role of an optimization variable. The parameter e is the positive elementary charge, $\hbar$ is the reduced Planck constant and

$$\mathcal{C}[f, f](t, \mathbf{k}) = \int_{\mathbb{R}^2} S(\mathbf{k}, \mathbf{k}') f(t, \mathbf{k}') (1 - f(t, \mathbf{k})) d\mathbf{k}' - \int_{\mathbb{R}^2} S(\mathbf{k}', \mathbf{k}) f(t, \mathbf{k}) (1 - f(t, \mathbf{k}')) d\mathbf{k}'$$

is the collision term. More details about the semiclassical Boltzmann equation have been already discussed in Chapter 1.

We would like to define an optimization problem in which the electron distribution is forced to assume a given probability density $\varphi(\mathbf{k})$ at the final time T , in the meanwhile it is also constrained to follow, in average, a certain trajectory $\theta(t, \mathbf{k})$ and minimizing also the cost of the control. More precisely, we would like to minimize the functional

$$J(f, u) = \int_0^T \int_{\mathbb{R}^2} \theta(t, \mathbf{k}) f(t, \mathbf{k}) d\mathbf{k} dt + \int_{\mathbb{R}^2} \varphi(\mathbf{k}) f_T(\mathbf{k}) d\mathbf{k} + \frac{\nu}{2} \|\mathbf{u}\|_{H_T^1},$$

where

$$\|\mathbf{u}\|_{H_T^1} = \int_0^T |\mathbf{u}(t)|^2 dt + \int_0^T \left| \frac{d}{dt} \mathbf{u}(t) \right|^2 dt$$

subject to the above mentioned differential constraint with the initial condition

$$f(0, \mathbf{k}) = f_0(\mathbf{k}).$$

The functional J represents the purpose of the optimization problem. This functional arises from the minimum attention control notion, see for example [16]. We call the first term the tracking term, the second term represents the final observation, and the last term denotes the costs of the control with a control weight $\nu > 0$. About the tracking term, the function θ represents an attracting potential for the electrons wave vectors.

Specifically, let us denote with $\mathbf{k}_d(t)$ a (time-dependent) desired profile confining the wave vectors of electrons. Then, we may choose $\theta(\mathbf{k}, t) = \Theta(|\mathbf{k} - \mathbf{k}_d(t)|)$ such that the global minimum of the tracking part is achieved when all particles have wave vectors $\mathbf{k}_d$. Similarly, the final observation term can be defined as $\varphi(\mathbf{k}) = \Phi(|\mathbf{k} - \mathbf{k}_T|)$, which may correspond to the requirement that, in average, the wave vectors of the particles at final time is close to $\mathbf{k}_T$. In general, we require that θ and φ are bounded from below and locally convex in the neighbourhood of $\mathbf{k}_d$ and $\mathbf{k}_T$, respectively.

6.1.1 The optimality system

In this section, we discuss the optimality system using the Lagrange framework. If we assume Fréchet differentiability, we can introduce the Lagrangian of the system, that writes

$$\mathcal{L}(f, \mathbf{u}, q) = J(f, \mathbf{u}) + \int_0^T \int_{\mathbb{R}^2} \left(\frac{\partial f}{\partial t} + \mathbf{u} \cdot \nabla_{\mathbf{k}} f - \mathcal{C}[f, f] \right) q(t, \mathbf{k}) d\mathbf{k} dt$$

The Gateaux derivative with respect to q writes

$$\begin{aligned} \nabla_q \mathcal{L} &= \lim_{h \rightarrow 0^+} \frac{1}{h} [\mathcal{L}(f, \mathbf{u}, q + h\delta q) - \mathcal{L}(f, \mathbf{u}, q)] \\ &= \lim_{h \rightarrow 0^+} \frac{1}{h} \left[\int_0^T \int_{\mathbb{R}^2} \left(\frac{\partial f}{\partial t} + \mathbf{u} \cdot \nabla_{\mathbf{k}} f - \mathcal{C}[f, f] \right) (q + h\delta q) d\mathbf{k} dt \right. \\ &\quad \left. - \int_0^T \int_{\mathbb{R}^2} \left(\frac{\partial f}{\partial t} + \mathbf{u} \cdot \nabla_{\mathbf{k}} f - \mathcal{C}[f, f] \right) q d\mathbf{k} dt \right] \\ &= \int_0^T \int_{\mathbb{R}^2} \left(\frac{\partial f}{\partial t} + \mathbf{u} \cdot \nabla_{\mathbf{k}} f - \mathcal{C}[f, f] \right) \delta q d\mathbf{k} dt \end{aligned}$$

By imposing it has to be zero $\forall \delta q(t, \mathbf{k})$ then

$$\frac{\partial f}{\partial t} + \mathbf{u} \cdot \nabla_{\mathbf{k}} f - \mathcal{C}[f, f] = 0.$$

The Gateaux derivative with respect to $\mathbf{u}$ writes

$$\begin{aligned} \nabla_{\mathbf{u}} \mathcal{L} &= \lim_{h \rightarrow 0^+} \frac{1}{h} [\mathcal{L}(f, \mathbf{u} + h\delta \mathbf{u}, q) - \mathcal{L}(f, \mathbf{u}, q)] \\ &= \lim_{h \rightarrow 0^+} \frac{1}{h} \left[\frac{\nu}{2} \|\mathbf{u} + h\delta \mathbf{u}\|_{H_T^1}^2 - \frac{\nu}{2} \|\mathbf{u}\|_{H_T^1}^2 \right. \\ &\quad \left. + \int_0^T \int_{\mathbb{R}^2} \left(\frac{\partial f}{\partial t} + (\mathbf{u} + h\delta \mathbf{u}) \cdot \nabla_{\mathbf{k}} f - \mathcal{C}[f, f] \right) q d\mathbf{k} dt \right. \\ &\quad \left. - \int_0^T \int_{\mathbb{R}^2} \left(\frac{\partial f}{\partial t} + \mathbf{u} \cdot \nabla_{\mathbf{k}} f - \mathcal{C}[f, f] \right) q d\mathbf{k} dt \right] \end{aligned}$$

Since

$$\begin{aligned}\|\mathbf{u} + h\delta\mathbf{u}\|_{H_T^1} &= \int_0^T |\mathbf{u}(t) + h\delta\mathbf{u}(t)|^2 dt + \int_0^T \left| \frac{d}{dt}(\mathbf{u}(t) + h\delta\mathbf{u}(t)) \right|^2 dt \\ &= \int_0^T \mathbf{u}(t)^2 + 2h\mathbf{u}(t) \cdot \delta\mathbf{u}(t) + h^2\delta\mathbf{u}(t)^2 dt + \int_0^T \left| \frac{d}{dt}\mathbf{u}(t) \right|^2 dt \\ &\quad + 2h \frac{d\mathbf{u}(t)}{dt} \cdot \frac{d\delta\mathbf{u}(t)}{dt} + h^2 \left| \frac{d}{dt}\delta\mathbf{u}(t) \right|^2 dt\end{aligned}$$

we get

$$\begin{aligned}\nabla_{\mathbf{u}}\mathcal{L} &= \nu \int_0^T \mathbf{u} \cdot \delta\mathbf{u} dt + \nu \int_0^T \frac{d\mathbf{u}(t)}{dt} \cdot \frac{d\delta\mathbf{u}(t)}{dt} dt + \int_0^T \int_{\mathbb{R}^2} (\delta\mathbf{u} \cdot \nabla_{\mathbf{k}} f) q d\mathbf{k} dt \\ &= \nu \int_0^T \mathbf{u} \cdot \delta\mathbf{u} dt + \nu \int_0^T \frac{d}{dt} \left(\frac{d\mathbf{u}}{dt} \cdot \delta\mathbf{u} \right) dt \\ &\quad - \nu \int_0^T \frac{d^2\mathbf{u}}{dt^2} \cdot \delta\mathbf{u} dt + \int_0^T \int_{\mathbb{R}^2} (\delta\mathbf{u} \cdot \nabla_{\mathbf{k}} f) q d\mathbf{k} dt \\ &= \nu \int_0^T \mathbf{u} \cdot \delta\mathbf{u} dt + \nu \left[\frac{d\mathbf{u}}{dt} \cdot \delta\mathbf{u} \right]_0^T - \nu \int_0^T \frac{d^2\mathbf{u}}{dt^2} \cdot \delta\mathbf{u} dt + \int_0^T \int_{\mathbb{R}^2} (\delta\mathbf{u} \cdot \nabla_{\mathbf{k}} f) q d\mathbf{k} dt \\ &= \int_0^T \delta\mathbf{u} \cdot \left(\nu\mathbf{u} - \nu \frac{d^2\mathbf{u}}{dt^2} + \int_{\mathbb{R}^2} q \nabla_{\mathbf{k}} f d\mathbf{k} \right)\end{aligned}$$

because we have set $\delta\mathbf{u}(0) = \delta\mathbf{u}(T) = \mathbf{0}$.

By imposing it has to be zero $\forall \delta\mathbf{u}(t)$ then

$$\nu\mathbf{u} - \nu \frac{d^2\mathbf{u}}{dt^2} + \int_{\mathbb{R}^2} q \nabla_{\mathbf{k}} f d\mathbf{k} = 0$$

The Gateaux derivative with respect to f writes

$$\begin{aligned}\nabla_f\mathcal{L} &= \lim_{h \rightarrow 0^+} \frac{1}{h} [\mathcal{L}(f + h\delta f, \mathbf{u}, q) - \mathcal{L}(f, \mathbf{u}, q)] \\ &= \lim_{h \rightarrow 0^+} \frac{1}{h} \left[\int_0^T \int_{\mathbb{R}^2} \theta(t, \mathbf{k}) (f(t, \mathbf{k}) + h\delta f(t, \mathbf{k})) d\mathbf{k} dt - \int_0^T \int_{\mathbb{R}^2} \theta(t, \mathbf{k}) f(t, \mathbf{k}) d\mathbf{k} dt \right. \\ &\quad + \int_0^T \int_{\mathbb{R}^2} \left(\frac{\partial f + h\delta f}{\partial t} + \mathbf{u} \cdot \nabla_{\mathbf{k}} (f + h\delta f) - \mathcal{C}[f + h\delta f, f + h\delta f] \right) q d\mathbf{k} dt \\ &\quad \left. - \int_0^T \int_{\mathbb{R}^2} \left(\frac{\partial f}{\partial t} + \mathbf{u} \cdot \nabla_{\mathbf{k}} f - \mathcal{C}[f, f] \right) q d\mathbf{k} dt \right].\end{aligned}$$

Since:

$$\begin{aligned}
\int_0^T \int_{\mathbb{R}^2} \frac{\partial \delta f}{\partial t} q \, d\mathbf{k} \, dt &= \int_{\mathbb{R}^2} [q \delta f]_0^T \, d\mathbf{k} - \int_0^T \int_{\mathbb{R}^2} \frac{\partial q}{\partial t} \delta f \, d\mathbf{k} \, dt \\
&= \int_{\mathbb{R}^2} q(T, \mathbf{k}) \delta f(T, \mathbf{k}) \, d\mathbf{k} - \int_{\mathbb{R}^2} q(0, \mathbf{k}) \delta f(0, \mathbf{k}) \, d\mathbf{k} - \int_0^T \int_{\mathbb{R}^2} \frac{\partial q}{\partial t} \delta f \, d\mathbf{k} \, dt \\
&= \int_{\mathbb{R}^2} q(T, \mathbf{k}) \delta f(T, \mathbf{k}) \, d\mathbf{k} - \int_0^T \int_{\mathbb{R}^2} \frac{\partial q}{\partial t} \delta f \, d\mathbf{k} \, dt
\end{aligned}$$

where the last step is obtained because $\delta f(0, \mathbf{k}) = 0$.

$$\int_0^T \int_{\mathbb{R}^2} (\mathbf{u} \cdot \nabla_{\mathbf{k}} f) q \, d\mathbf{k} \, dt = - \int_0^T \int_{\mathbb{R}^2} (\mathbf{u} \cdot \nabla_{\mathbf{k}} q) \delta f \, d\mathbf{k} \, dt$$

because of the exponential decay of f for $|\mathbf{k}| \rightarrow +\infty$.

By putting everything together we have

$$\begin{aligned}
\nabla_f \mathcal{L} &= \int_0^T \int_{\mathbb{R}^2} \theta(t, \mathbf{k}) \delta f(t, \mathbf{k}) \, d\mathbf{k} \, dt \\
&\quad + \int_{\mathbb{R}^2} q(T, \mathbf{k}) \delta f(T, \mathbf{k}) \, d\mathbf{k} - \int_0^T \int_{\mathbb{R}^2} \frac{\partial q}{\partial t} \delta f \, d\mathbf{k} \, dt - \int_0^T \int_{\mathbb{R}^2} (\mathbf{u} \cdot \nabla_{\mathbf{k}} q) \delta f \, d\mathbf{k} \, dt \\
&\quad - \lim_{h \rightarrow 0^+} \frac{1}{h} \left[\int_0^T \int_{\mathbb{R}^2} (\mathcal{C}[f + h\delta f, f + h\delta f] - \mathcal{C}[f, f]) q \, d\mathbf{k} \, dt \right].
\end{aligned}$$

Let us expand the collision term

$$\begin{aligned}
&\mathcal{C}[f + h\delta f, f + h\delta f] - \mathcal{C}[f, f] \\
&= \int_{\mathbb{R}^2} S(\mathbf{k}, \mathbf{k}') (f + h\delta f)(t, \mathbf{k}') (1 - (f + h\delta f)(t, \mathbf{k})) \, d\mathbf{k}' \\
&\quad - \int_{\mathbb{R}^2} S(\mathbf{k}', \mathbf{k}) (f + h\delta f)(t, \mathbf{k}) (1 - (f + h\delta f)(t, \mathbf{k}')) \, d\mathbf{k}' \\
&\quad - \int_{\mathbb{R}^2} S(\mathbf{k}, \mathbf{k}') f(t, \mathbf{k}') (1 - f(t, \mathbf{k})) \, d\mathbf{k}' + \int_{\mathbb{R}^2} S(\mathbf{k}', \mathbf{k}) f(t, \mathbf{k}) (1 - f(t, \mathbf{k}')) \, d\mathbf{k}' \\
&= \int_{\mathbb{R}^2} S(\mathbf{k}, \mathbf{k}') (f(\mathbf{k}') (1 - f(\mathbf{k})) - hf(\mathbf{k}') \delta f(\mathbf{k}) + h\delta f(\mathbf{k}') (1 - f(\mathbf{k})) - h^2 \delta f(\mathbf{k}') \delta f(\mathbf{k})) \, d\mathbf{k}' \\
&\quad - \int_{\mathbb{R}^2} S(\mathbf{k}', \mathbf{k}) (f(\mathbf{k}) (1 - f(\mathbf{k}')) - hf(\mathbf{k}) \delta f(\mathbf{k}') + h\delta f(\mathbf{k}) (1 - f(\mathbf{k}')) - h^2 \delta f(\mathbf{k}) \delta f(\mathbf{k}')) \, d\mathbf{k}' \\
&\quad - \int_{\mathbb{R}^2} S(\mathbf{k}, \mathbf{k}') f(t, \mathbf{k}') (1 - f(t, \mathbf{k})) \, d\mathbf{k}' + \int_{\mathbb{R}^2} S(\mathbf{k}', \mathbf{k}) f(t, \mathbf{k}) (1 - f(t, \mathbf{k}')) \, d\mathbf{k}' \\
&= \int_{\mathbb{R}^2} S(\mathbf{k}, \mathbf{k}') (-hf(\mathbf{k}') \delta f(\mathbf{k}) + h\delta f(\mathbf{k}') (1 - f(\mathbf{k})) - h^2 \delta f(\mathbf{k}') \delta f(\mathbf{k})) \, d\mathbf{k}' \\
&\quad - \int_{\mathbb{R}^2} S(\mathbf{k}', \mathbf{k}) (-hf(\mathbf{k}) \delta f(\mathbf{k}') + h\delta f(\mathbf{k}) (1 - f(\mathbf{k}')) - h^2 \delta f(\mathbf{k}) \delta f(\mathbf{k}')) \, d\mathbf{k}'.
\end{aligned}$$

Then

$$\begin{aligned}
& \lim_{h \rightarrow 0^+} \frac{1}{h} [\mathcal{C}[f + h\delta f, f + h\delta f] - \mathcal{C}[f, f]] q \\
&= \left[\int_{\mathbb{R}^2} S(\mathbf{k}, \mathbf{k}') (-f(\mathbf{k}')\delta f(\mathbf{k}) + \delta f(\mathbf{k}')(1 - f(\mathbf{k}))) d\mathbf{k}' \right. \\
&\quad \left. - \int_{\mathbb{R}^2} S(\mathbf{k}', \mathbf{k}) (-f(\mathbf{k})\delta f(\mathbf{k}') + \delta f(\mathbf{k})(1 - f(\mathbf{k}')))) d\mathbf{k}' \right] q \\
&= \left[\int_{\mathbb{R}^2} S(\mathbf{k}, \mathbf{k}') (-f(\mathbf{k}')\delta f(\mathbf{k}) - \delta f(\mathbf{k}')f(\mathbf{k})) d\mathbf{k}' \right. \\
&\quad \left. - \int_{\mathbb{R}^2} S(\mathbf{k}', \mathbf{k}) (-f(\mathbf{k})\delta f(\mathbf{k}') - \delta f(\mathbf{k})f(\mathbf{k}')) d\mathbf{k}' \right. \\
&\quad \left. + \int_{\mathbb{R}^2} S(\mathbf{k}, \mathbf{k}')\delta f(\mathbf{k}') d\mathbf{k}' - \int_{\mathbb{R}^2} S(\mathbf{k}', \mathbf{k})\delta f(\mathbf{k}) d\mathbf{k}' \right] q
\end{aligned}$$

Now let us consider the quantity

$$\begin{aligned}
& \int_{\mathbb{R}^2} \left[\int_{\mathbb{R}^2} S(\mathbf{k}, \mathbf{k}') (-f(\mathbf{k}')\delta f(\mathbf{k}) - \delta f(\mathbf{k}')f(\mathbf{k})) d\mathbf{k}' \right. \\
&\quad \left. - \int_{\mathbb{R}^2} S(\mathbf{k}', \mathbf{k}) (-f(\mathbf{k})\delta f(\mathbf{k}') - \delta f(\mathbf{k})f(\mathbf{k}')) d\mathbf{k}' \right. \\
&\quad \left. + \int_{\mathbb{R}^2} S(\mathbf{k}, \mathbf{k}')\delta f(\mathbf{k}') d\mathbf{k}' - \int_{\mathbb{R}^2} S(\mathbf{k}', \mathbf{k})\delta f(\mathbf{k}) d\mathbf{k}' \right] q(t, \mathbf{k}) d\mathbf{k}
\end{aligned}$$

and manipulate it obtaining

$$\begin{aligned}
& \int_{\mathbb{R}^2} \left[\int_{\mathbb{R}^2} S(\mathbf{k}, \mathbf{k}') (-f(\mathbf{k}')\delta f(\mathbf{k}) - \delta f(\mathbf{k}')f(\mathbf{k})) d\mathbf{k}' \right. \\
&\quad \left. - \int_{\mathbb{R}^2} S(\mathbf{k}', \mathbf{k}) (-f(\mathbf{k})\delta f(\mathbf{k}') - \delta f(\mathbf{k})f(\mathbf{k}')) d\mathbf{k}' \right. \\
&\quad \left. + \int_{\mathbb{R}^2} S(\mathbf{k}, \mathbf{k}')\delta f(\mathbf{k}') d\mathbf{k}' - \int_{\mathbb{R}^2} S(\mathbf{k}', \mathbf{k})\delta f(\mathbf{k}) d\mathbf{k}' \right] q(t, \mathbf{k}) d\mathbf{k} \\
&= \int_{\mathbb{R}^2} \delta f(\mathbf{k}) \left[\int_{\mathbb{R}^2} S(\mathbf{k}, \mathbf{k}') (-f(\mathbf{k}')) d\mathbf{k}' - \int_{\mathbb{R}^2} S(\mathbf{k}', \mathbf{k}) (-f(\mathbf{k}')) d\mathbf{k}' \right. \\
&\quad \left. - \int_{\mathbb{R}^2} S(\mathbf{k}', \mathbf{k}) d\mathbf{k}' \right] q(t, \mathbf{k}) d\mathbf{k} \\
&\quad + \int_{\mathbb{R}^2} \left[\int_{\mathbb{R}^2} S(\mathbf{k}, \mathbf{k}') (-\delta f(\mathbf{k}')f(\mathbf{k})) d\mathbf{k}' - \int_{\mathbb{R}^2} S(\mathbf{k}', \mathbf{k}) (-f(\mathbf{k})\delta f(\mathbf{k}')) d\mathbf{k}' \right. \\
&\quad \left. + \int_{\mathbb{R}^2} S(\mathbf{k}, \mathbf{k}')\delta f(\mathbf{k}') d\mathbf{k}' \right] q(t, \mathbf{k}) d\mathbf{k}
\end{aligned}$$

Now in the first integral we relabel $\mathbf{k}' = \bar{\mathbf{k}}$ and in the second one $\mathbf{k}' = \mathbf{k}$, $\mathbf{k} = \bar{\mathbf{k}}$ getting

$$\begin{aligned}
& \int_{\mathbb{R}^2} \delta f(\mathbf{k}) \left[\int_{\mathbb{R}^2} S(\mathbf{k}, \bar{\mathbf{k}}) (-f(\bar{\mathbf{k}})) d\bar{\mathbf{k}} - \int_{\mathbb{R}^2} S(\bar{\mathbf{k}}, \mathbf{k}) (-f(\bar{\mathbf{k}})) d\bar{\mathbf{k}} - \int_{\mathbb{R}^2} S(\bar{\mathbf{k}}, \mathbf{k}) d\bar{\mathbf{k}} \right] q(t, \mathbf{k}) d\mathbf{k} \\
& + \int_{\mathbb{R}^2} \left[\int_{\mathbb{R}^2} S(\bar{\mathbf{k}}, \mathbf{k}) (-\delta f(\mathbf{k}) f(\bar{\mathbf{k}})) d\mathbf{k} - \int_{\mathbb{R}^2} S(\mathbf{k}, \bar{\mathbf{k}}) (-f(\bar{\mathbf{k}}) \delta f(\mathbf{k})) d\mathbf{k} \right. \\
& \left. + \int_{\mathbb{R}^2} S(\bar{\mathbf{k}}, \mathbf{k}) \delta f(\mathbf{k}) d\mathbf{k} \right] q(t, \bar{\mathbf{k}}) d\bar{\mathbf{k}} \\
& = \int_{\mathbb{R}^2} \delta f(\mathbf{k}) \left[\int_{\mathbb{R}^2} S(\mathbf{k}, \bar{\mathbf{k}}) (-f(\bar{\mathbf{k}})) q(t, \mathbf{k}) d\bar{\mathbf{k}} - \int_{\mathbb{R}^2} S(\bar{\mathbf{k}}, \mathbf{k}) (-f(\bar{\mathbf{k}})) q(t, \mathbf{k}) d\bar{\mathbf{k}} \right. \\
& \left. - \int_{\mathbb{R}^2} S(\bar{\mathbf{k}}, \mathbf{k}) q(t, \mathbf{k}) d\bar{\mathbf{k}} \right] d\mathbf{k} \\
& + \int_{\mathbb{R}^2} \delta f(\mathbf{k}) \left[\int_{\mathbb{R}^2} S(\bar{\mathbf{k}}, \mathbf{k}) (-f(\bar{\mathbf{k}})) q(t, \bar{\mathbf{k}}) d\bar{\mathbf{k}} - \int_{\mathbb{R}^2} S(\mathbf{k}, \bar{\mathbf{k}}) (-f(\bar{\mathbf{k}})) q(t, \bar{\mathbf{k}}) d\bar{\mathbf{k}} \right. \\
& \left. + \int_{\mathbb{R}^2} S(\bar{\mathbf{k}}, \mathbf{k}) q(t, \bar{\mathbf{k}}) d\bar{\mathbf{k}} \right] d\mathbf{k} \\
& = \int_{\mathbb{R}^2} \delta f(\mathbf{k}) \left[\int_{\mathbb{R}^2} S(\mathbf{k}, \bar{\mathbf{k}}) (-f(\bar{\mathbf{k}})) q(t, \mathbf{k}) d\bar{\mathbf{k}} - \int_{\mathbb{R}^2} S(\bar{\mathbf{k}}, \mathbf{k}) (-f(\bar{\mathbf{k}})) q(t, \mathbf{k}) d\bar{\mathbf{k}} \right. \\
& \left. - \int_{\mathbb{R}^2} S(\bar{\mathbf{k}}, \mathbf{k}) q(t, \mathbf{k}) d\bar{\mathbf{k}} + \int_{\mathbb{R}^2} S(\bar{\mathbf{k}}, \mathbf{k}) (-f(\bar{\mathbf{k}})) q(t, \bar{\mathbf{k}}) d\bar{\mathbf{k}} \right. \\
& \left. - \int_{\mathbb{R}^2} S(\mathbf{k}, \bar{\mathbf{k}}) (-f(\bar{\mathbf{k}})) q(t, \bar{\mathbf{k}}) d\bar{\mathbf{k}} + \int_{\mathbb{R}^2} S(\bar{\mathbf{k}}, \mathbf{k}) q(t, \bar{\mathbf{k}}) d\bar{\mathbf{k}} \right] d\mathbf{k} \\
& = \int_{\mathbb{R}^2} \delta f(\mathbf{k}) \left[\int_{\mathbb{R}^2} S(\mathbf{k}, \bar{\mathbf{k}}) (-f(\bar{\mathbf{k}})) q(t, \mathbf{k}) d\bar{\mathbf{k}} - \int_{\mathbb{R}^2} S(\bar{\mathbf{k}}, \mathbf{k}) (1 - f(\bar{\mathbf{k}})) q(t, \mathbf{k}) d\bar{\mathbf{k}} \right. \\
& \left. + \int_{\mathbb{R}^2} S(\bar{\mathbf{k}}, \mathbf{k}) (1 - f(\bar{\mathbf{k}})) q(t, \bar{\mathbf{k}}) d\bar{\mathbf{k}} - \int_{\mathbb{R}^2} S(\mathbf{k}, \bar{\mathbf{k}}) (-f(\bar{\mathbf{k}})) q(t, \bar{\mathbf{k}}) d\bar{\mathbf{k}} \right] d\mathbf{k},
\end{aligned}$$

relabeling back $\bar{\mathbf{k}} = \mathbf{k}'$ we have

$$\begin{aligned}
& \int_{\mathbb{R}^2} \delta f(\mathbf{k}) \left[\int_{\mathbb{R}^2} S(\mathbf{k}, \mathbf{k}') (-f(\mathbf{k}')) q(t, \mathbf{k}) d\mathbf{k}' - \int_{\mathbb{R}^2} S(\mathbf{k}', \mathbf{k}) (1 - f(\mathbf{k}')) q(t, \mathbf{k}) d\mathbf{k}' \right. \\
& \left. + \int_{\mathbb{R}^2} S(\mathbf{k}', \mathbf{k}) (1 - f(\mathbf{k}')) q(t, \mathbf{k}') d\mathbf{k}' - \int_{\mathbb{R}^2} S(\mathbf{k}, \mathbf{k}') (-f(\mathbf{k}')) q(t, \mathbf{k}') d\mathbf{k}' \right] d\mathbf{k}, \\
& = \int_{\mathbb{R}^2} \delta f(\mathbf{k}) \left[- \int_{\mathbb{R}^2} S(\mathbf{k}, \mathbf{k}') f(\mathbf{k}') (q(t, \mathbf{k}) - q(t, \mathbf{k}')) d\mathbf{k}' \right. \\
& \left. - \int_{\mathbb{R}^2} S(\mathbf{k}', \mathbf{k}) (1 - f(\mathbf{k}')) (q(t, \mathbf{k}) - q(t, \mathbf{k}')) d\mathbf{k}' \right] d\mathbf{k},
\end{aligned}$$

Finally we have

$$\begin{aligned}
\nabla_f \mathcal{L} &= \int_0^T \int_{\mathbb{R}^2} \theta(t, \mathbf{k}) \delta f \, d\mathbf{k} \, dt \\
&+ \int_{\mathbb{R}^2} q(T, \mathbf{k}) \delta f(T, \mathbf{k}) \, d\mathbf{k} - \int_0^T \int_{\mathbb{R}^2} \frac{\partial q}{\partial t} \delta f \, d\mathbf{k} \, dt - \int_0^T \int_{\mathbb{R}^2} (\mathbf{u} \cdot \nabla_{\mathbf{k}} q) \delta f \, d\mathbf{k} \, dt \\
&- \int_0^T \int_{\mathbb{R}^2} \delta f(t, \mathbf{k}) \left[- \int_{\mathbb{R}^2} S(\mathbf{k}, \mathbf{k}') f(\mathbf{k}') (q(t, \mathbf{k}) - q(t, \mathbf{k}')) \, d\mathbf{k}' \right. \\
&\quad \left. - \int_{\mathbb{R}^2} S(\mathbf{k}', \mathbf{k}) (1 - f(\mathbf{k}')) (q(t, \mathbf{k}) - q(t, \mathbf{k}')) \, d\mathbf{k}' \right] d\mathbf{k} \\
&= \int_0^T \int_{\mathbb{R}^2} \left[\theta(t, \mathbf{k}) - \frac{\partial q}{\partial t} - \mathbf{u} \cdot \nabla_{\mathbf{k}} q + \int_{\mathbb{R}^2} S(\mathbf{k}, \mathbf{k}') f(\mathbf{k}') (q(t, \mathbf{k}) - q(t, \mathbf{k}')) \, d\mathbf{k}' \right. \\
&\quad \left. + \int_{\mathbb{R}^2} S(\mathbf{k}', \mathbf{k}) (1 - f(\mathbf{k}')) (q(t, \mathbf{k}) - q(t, \mathbf{k}')) \, d\mathbf{k}' \right] \delta f \, d\mathbf{k} \, dt \\
&+ \int_{\mathbb{R}^2} [\beta(f(T, \mathbf{k}) - f_T(\mathbf{k})) + q(T, \mathbf{k})] \delta f(T, \mathbf{k}) \, d\mathbf{k}.
\end{aligned}$$

Then by imposing $\nabla_f \mathcal{L} = 0$ for all $\delta f(t, \mathbf{k})$ we obtain the adjoint equation

$$\begin{aligned}
& - \frac{\partial q}{\partial t} - \mathbf{u} \cdot \nabla_{\mathbf{k}} q + \int_{\mathbb{R}^2} S(\mathbf{k}, \mathbf{k}') f(\mathbf{k}') (q(t, \mathbf{k}) - q(t, \mathbf{k}')) \, d\mathbf{k}' \\
& + \int_{\mathbb{R}^2} S(\mathbf{k}', \mathbf{k}) (1 - f(\mathbf{k}')) (q(t, \mathbf{k}) - q(t, \mathbf{k}')) \, d\mathbf{k}' + \theta(t, \mathbf{k}) = 0
\end{aligned}$$

or equivalently

$$- \frac{\partial q}{\partial t} - \mathbf{u} \cdot \nabla_{\mathbf{k}} q + C^*[f, q](t, \mathbf{k}) + \theta(t, \mathbf{k}) = 0$$

with

$$\begin{aligned}
C^*[f, q](t, \mathbf{k}) &= \int_{\mathbb{R}^2} S(\mathbf{k}, \mathbf{k}') f(\mathbf{k}') (q(t, \mathbf{k}) - q(t, \mathbf{k}')) \, d\mathbf{k}' \\
&+ \int_{\mathbb{R}^2} S(\mathbf{k}', \mathbf{k}) (1 - f(\mathbf{k}')) (q(t, \mathbf{k}) - q(t, \mathbf{k}')) \, d\mathbf{k}'.
\end{aligned}$$

6.2 Numerical method

We suppose that $\mathbf{u}$ is directed along k_x , that is

$$\mathbf{u}(t) = \left(-\frac{e}{\hbar} E(t), 0 \right). \tag{6.2}$$

Then the optimality system writes

$$\begin{cases} \frac{\partial f}{\partial t} - \frac{e}{\hbar} E(t) \frac{\partial f}{\partial k_x} = \mathcal{C}[f, f] \\ -\frac{\partial q}{\partial t} + \frac{e}{\hbar} E(t) \frac{\partial q}{\partial k_x} + C^*[f, q](t, \mathbf{k}) + \theta(t, \mathbf{k}) = 0 \\ \frac{d^2 E(t)}{dt^2} - E(t) = -\frac{\hbar}{e} \frac{1}{v} \int_{\mathbb{R}^2} q \frac{\partial f}{\partial k_x} f d\mathbf{k} \end{cases} \quad (6.3)$$

where the first equation is called forward equation, the second equation is the adjoint and the last one is the gradient. As initial condition for f we take the Fermi-Dirac distribution

$$f(0, \mathbf{k}) = \frac{1}{1 + \exp\left(\frac{\varepsilon(\mathbf{k}) - \varepsilon_F}{k_B T}\right)} \quad (6.4)$$

where $\varepsilon(\mathbf{k}) = \hbar v_F |\mathbf{k}|$. And as terminal condition for q a shifted Fermi-Dirac

$$\varphi(\mathbf{k}) = \frac{1}{1 + \exp\left(\frac{\varepsilon(\mathbf{k} - \mathbf{k}_T) - \varepsilon_F}{k_B T}\right)} \quad (6.5)$$

About θ we may set for example

$$\theta(t, \mathbf{k}) = \frac{1}{1 + \exp\left(\frac{\varepsilon(\mathbf{k} - \mathbf{k}_d(t)) - \varepsilon_F}{k_B T}\right)} \quad (6.6)$$

with

$$\mathbf{k}_d(t) = \mathbf{a}t^2 + \mathbf{b}t + \mathbf{c} \quad (6.7)$$

satisfying $\mathbf{k}_d(0) = \mathbf{0}$ and $\mathbf{k}_d(T) = \mathbf{k}_T$.

6.2.1 The discontinuous Galerkin method

Since we expect an exponential decay of f , as $|\mathbf{k}| \rightarrow +\infty$, it is reasonable to choose a compact domain $\Omega \subseteq \mathbb{R}^2$, such that $f(t, \mathbf{k}) \approx 0$, for every $\mathbf{k} \notin \Omega$ and $t > 0$.

As in , let us introduce a finite decomposition $\{C_\alpha : \alpha = 1, 2, \dots, N\}$ of the domain Ω , with the C_α 's open sets such that

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

We assume a constant approximation for each distribution function f, q in every cell C_α . If we denote by χ_α the characteristic function relative to the cell C_α , then

$$\begin{aligned} f(t, \mathbf{k}) \approx f^\alpha(t), \forall \mathbf{k} \in C_\alpha &\iff f(t, \mathbf{k}) \approx \sum_{\alpha=1}^N f^\alpha(t) \chi_\alpha(\mathbf{k}), \forall \mathbf{k} \in \bigcup_{\alpha=1}^N C_\alpha \\ q(t, \mathbf{k}) \approx q^\alpha(t), \forall \mathbf{k} \in C_\alpha &\iff q(t, \mathbf{k}) \approx \sum_{\alpha=1}^N q^\alpha(t) \chi_\alpha(\mathbf{k}), \forall \mathbf{k} \in \bigcup_{\alpha=1}^N C_\alpha \end{aligned}$$

A set of partial differential equations is now derived from the Boltzmann equations. The new unknowns are the $f^\alpha(t)$ and $q^\alpha(t)$ instead of the distribution functions $f(t, \mathbf{k})$ and $q(t, \mathbf{k})$. Formally integrating over each cell C_α , we obtain

$$\int_{C_\alpha} \frac{\partial f}{\partial t} d\mathbf{k} - \int_{C_\alpha} \frac{e}{\hbar} \mathbf{E} \cdot \nabla_{\mathbf{k}} f d\mathbf{k} = \int_{C_\alpha} \mathcal{C}[f, f] d\mathbf{k}. \quad (6.8)$$

$$- \int_{C_\alpha} \frac{\partial q}{\partial t} d\mathbf{k} + \int_{C_\alpha} \frac{e}{\hbar} \mathbf{E} \cdot \nabla_{\mathbf{k}} q d\mathbf{k} + \int_{C_\alpha} \mathcal{C}^*[f, q] d\mathbf{k} + \int_{C_\alpha} \theta(t, \mathbf{k}) d\mathbf{k} = 0. \quad (6.9)$$

6.2.2 Numerical flux

The first integral of Eq.s (6.8),(6.9) can be approximated easily; in fact we have

$$\begin{aligned} \int_{C_\alpha} \frac{\partial f}{\partial t} d\mathbf{k} &\approx \text{meas}(C_\alpha) \frac{\partial f^\alpha}{\partial t}(t) \\ \int_{C_\alpha} \frac{\partial q}{\partial t} d\mathbf{k} &\approx \text{meas}(C_\alpha) \frac{\partial q^\alpha}{\partial t}(t) \end{aligned}$$

where $\text{meas}(C_\alpha)$ is the measure (area) of the cell C_α .

The integral involving the electric field is transformed by using the Gauss theorem,

$$\begin{aligned} -\frac{e}{\hbar} \mathbf{E} \cdot \int_{C_\alpha} \nabla_{\mathbf{k}} f d\mathbf{k} &= -\frac{e}{\hbar} \mathbf{E} \cdot \int_{\partial C_\alpha} f \mathbf{n} d\sigma. \\ \frac{e}{\hbar} \mathbf{E} \cdot \int_{C_\alpha} \nabla_{\mathbf{k}} q d\mathbf{k} &= \frac{e}{\hbar} \mathbf{E} \cdot \int_{\partial C_\alpha} q \mathbf{n} d\sigma. \end{aligned}$$

Since the approximation of f and q is not defined on the boundary of the cells, we must introduce a numerical flux, that furnishes reasonable values of f_s on every ∂C_α . We have used a reconstruction of the fluxes based on a Min-Mod slope limiter, as in [25].

We conclude this section with the treatment of the term arising from the collision operator. If $\mathbf{k} \in C_\alpha$, then we have

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

So, defining

$$A^{\alpha,\beta} = \int_{C_\alpha} \left[\int_{C_\beta} S(\mathbf{k}', \mathbf{k}) d\mathbf{k}' \right] d\mathbf{k}, \quad (6.10)$$

it is immediate to verify that

$$\int_{C_\alpha} \mathcal{C}(f, f) d\mathbf{k} \approx \sum_{\beta=1}^N \left[A^{\beta,\alpha} (1 - f^\alpha(t)) f^\beta(t) - A^{\alpha,\beta} f^\alpha(t) (1 - f^\beta(t)) \right]. \quad (6.11)$$

Analogously, for the collision term of the adjoint equation, we get

$$\int_{C_\alpha} \mathcal{C}^*(f, q) d\mathbf{k} \approx \sum_{\beta=1}^N \left[A^{\alpha,\beta} f^\beta(t) (q^\alpha(t) - q^\beta(t)) + A^{\beta,\alpha} (1 - f^\beta(t)) (q^\alpha(t) - q^\beta(t)) \right]. \quad (6.12)$$

6.2.3 Numerical optimization procedure

In this section, we present the optimization algorithm, we use to solve (6.3). We adopt a non-linear conjugated gradient method, see [15] for references. In Algorithm 6.2.1, the main structure of the procedure is given.

To initiate the optimization, the first guess $\mathbf{u}^0(t)$ of the control which is usually $\mathbf{u}^0(t) \equiv \mathbf{0}$, the initial condition of the forward equation $f_0(\mathbf{k})$, the potential corresponding to the terminal condition $\varphi(\mathbf{k})$ and the tracking potential $\theta(\mathbf{k}, t)$, are required.

The quantities tol , $n_{\max}$ are both positive and used for termination criteria. Since we do not impose constraints on the control function, we know from the first order optimality condition that the norm of the gradient has to be zero at the optimum. Therefore, we stop the algorithm, if $\|g^n\|_{H_T^1}$ is smaller than a threshold tol , which is close to zero. An additional termination criterion is a maximum number of iterations $n_{\max}$.

Algorithm 6.2.1 Non-linear conjugated gradient scheme (nCG)

Require: $u^0(t)$, $f_0(\mathbf{k})$, $\varphi(\mathbf{k})$, $\theta(\mathbf{k}, t)$

Ensure: Optimal solution $\mathbf{u}^*(t)$ and corresponding state $f^*(\mathbf{k}, t)$

- 1: $n = 0$
 - 2: Assemble gradient $\psi^0(t)$ using Algorithm 6.2.2
 - 3: **while** $\|g^n\|_{H_T^1} > tol$ **and** $n < n_{\max}$ **do**
 - 4: Assemble reduced gradient $\psi^n(t)$ using Algorithm 6.2.2
 - 5: Use nCG-scheme for calculating new descent direction $\mathbf{d}^n$ (see [15])
 - 6: Apply an appropriate line-search algorithm to obtain suitable step-size α_n along $\mathbf{d}^n$
 - 7: Update control: $\mathbf{u}^{n+1} = \mathbf{u}^n + \alpha_n \mathbf{d}^n$
 - 8: Set $n = n + 1$
 - 9: **end while**
 - 10: **return** $(\mathbf{u}^n, f^n)$
-

In Algorithm 6.2.2, the procedure to calculate the gradient, needed in Algorithm 6.2.1, is given. It requires the current control $\mathbf{u}(t)$, the initial condition of the forward equation and the potentials φ , θ . During the calculation of the gradient, the forward and backward equations have to be solved by means of the DG method described in Section 6.2.1. Keep in mind that while solving the backward equation, the time reversing has to be taken into account.

Algorithm 6.2.2 Calculating gradient of reduced cost functional

Require: control $\mathbf{u}(t)$, $f_0(\mathbf{k})$, $\varphi(\mathbf{k})$, $\theta(\mathbf{k}, t)$

Ensure: reduced gradient $\nabla J_r(t)$

- 1: Solve forward equation by the DG method with inputs: $f_0(\mathbf{k})$, $\mathbf{u}(t)$
 - 2: Solve backward equation by the DG method with inputs: $-\varphi(\mathbf{k})$, $\mathbf{u}(T - t)$, $a_\theta(\mathbf{k}, T - t)$
 - 3: Assemble reduced gradient.
 - 4: **return** $\psi(t)$
-

We remark that just a theoretical study has been done. To complete the work, the proposed method have to be implemented and numerical results have to be examined. It will be part of a forthcoming publication.

Chapter 7

Further developments

In this chapter we would like to introduce two ongoing works. In Section 7.1 we present the problem of considering electron-electron interaction in the semiclassical Boltzmann equation. Some numerical results are obtained by means of Direct Simulation Monte Carlo approach [28]. In Section 7.2 we outline the problem of simulating a graphene based electron device modeling the charge transport with the semiclassical Boltzmann equation in the non homogeneous case. Some preliminary numerical results are obtained by the Discontinuous Galerkin method [80].

Both the works are still in preprint version and they have been presented at the 26th International Congress on Transport Theory (ICTT-26), held in Paris in September 2019.

7.1 The effect of electron-electron scattering in graphene

Charge transport in graphene may be described with good accuracy by the semiclassical Boltzmann equation. If $f(t, \mathbf{r}, \mathbf{k})$ is the distribution of electrons in the conduction band, by taking into account also the electron-electron interaction, it reads (see [101]):

$$\begin{aligned} \frac{\partial f(\mathbf{k}_1)}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{r}} f(\mathbf{k}_1) - \frac{e}{\hbar} \mathbf{E} \cdot \nabla_{\mathbf{k}_1} f(\mathbf{k}_1) = \\ = \sum_{\alpha, \mathbf{k}_1} [f(\mathbf{k}'_1) s_{\alpha}(\mathbf{k}'_1, \mathbf{k}_1) (1 - f(\mathbf{k}_1)) - f(\mathbf{k}_1) s_{\alpha}(\mathbf{k}_1, \mathbf{k}'_1) (1 - f(\mathbf{k}'_1))] + \\ + \sum_{\mathbf{k}'_1, \mathbf{k}_2, \mathbf{k}'_2} [f(\mathbf{k}'_1) f(\mathbf{k}'_2) s_{ee}(\mathbf{k}'_1, \mathbf{k}'_2, \mathbf{k}_1, \mathbf{k}_2) (1 - f(\mathbf{k}_1)) (1 - f(\mathbf{k}_2)) + \\ - f(\mathbf{k}_1) f(\mathbf{k}_2) s_{ee}(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}'_1, \mathbf{k}'_2) (1 - f(\mathbf{k}'_1)) (1 - f(\mathbf{k}'_2))] , \end{aligned}$$

where the only dependence on $\mathbf{k}$ is written to avoid an annoying notation. $s_{\alpha}(\mathbf{k}, \mathbf{k}')$ is the transition rate from the state $\mathbf{k}$ to $\mathbf{k}'$ due to the interaction with the α th phonon branch while $s_{ee}(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}'_1, \mathbf{k}'_2)$ is the transition rate among the states $\mathbf{k}_1 \rightarrow \mathbf{k}'_1$ e $\mathbf{k}_2 \rightarrow \mathbf{k}'_2$.

Following [55], the transition rate s_{ee} , obtained by means of the Fermi golden rule, is given by

$$s_{ee}(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}'_1, \mathbf{k}'_2) = \frac{2\pi}{\hbar} |M|^2 \delta(\varepsilon(\mathbf{k}'_1) + \varepsilon(\mathbf{k}'_2) - \varepsilon(\mathbf{k}_1) - \varepsilon(\mathbf{k}_2)),$$

where the dispersion relation around the Dirac points of the first Brillouin zone is assumed to be $\varepsilon(\mathbf{k}) = \hbar v_F |\mathbf{k}|$. The generic element of the interaction matrix, is

$$|M|^2 = \frac{1}{2} \left[|V(q)|^2 + |V(q')|^2 - V(q)V(q') \right],$$

with

$$V(q) = \frac{2\pi e^2}{\epsilon(q)qA} \frac{1 + \cos(\phi_{\mathbf{k}_1, \mathbf{k}'_1})}{2} \frac{1 + \cos(\phi_{\mathbf{k}_2, \mathbf{k}'_2})}{2},$$

where $q = |\mathbf{k}_1 - \mathbf{k}'_1|$. In the above expressions $\phi_{\mathbf{k}, \mathbf{k}'}$ indicates the angle between $\mathbf{k}$ and $\mathbf{k}'$. For further details see [36], [93] e [14].

Under the hypothesis of *random-phase approximation* (valid for density $n \geq 10^{12} \text{cm}^{-2}$), the dielectric function $\epsilon(q)$ is given by ([43]):

$$\epsilon(q) = 1 + v_c(q)\Pi(q),$$

where $v_c(q) = 2\pi e^2 / \kappa q$, with κ (*background lattice dielectric constant*) which satisfies the relation $r_s = \frac{e^2}{\kappa \gamma} \sqrt{\frac{4}{g_s g_v}}$, Here $\gamma = \hbar v_F$, where g_s and g_v are the spin and valley degeneracy, and r_s a dimensionless constant (the *Wigner-Seitz radius*). If we introduce the function $\tilde{\Pi}(q) = \tilde{\Pi}^-(q) + \tilde{\Pi}^+(q)$, with

$$\tilde{\Pi}^-(q) = \frac{\pi q}{8k_F}$$

and

$$\tilde{\Pi}^+(q) = \begin{cases} 1 - \frac{\pi q}{8k_F} & \text{se } q < 2k_F \\ 1 - \frac{\sqrt{q^2 - 4k_F^2}}{2q} - \frac{q}{4k_F} \arcsin\left(\frac{2k_F}{q}\right) & \text{otherwise} \end{cases}$$

where $k_F = \sqrt{4\pi n / g_s g_v}$, n being the electron density, one has $\Pi(q) = D(E_F) \tilde{\Pi}(q)$. $D(\varepsilon) = \frac{g_v g_s |\varepsilon|}{2\pi \gamma^2}$ is the density of state. A more detailed discussion about the physical aspects can be found in [19] e [31].

7.1.1 Numerical results

The complexity of the electron-electron scattering makes very difficult the use of deterministic methods like finite difference approaches, e.g. WENO schemes, or discontinuous Galerkin methods, which provided very efficient when only the electron-phonon scattering is taken into account [25, 63]. The main issue to be tackled is the evaluation of the delta's present into the scattering rate.

The most viable method remains that based on a Direct Simulation Monte Carlo (DSMC). However in the presence of degeneracy effects, the standard DSMC approach fails to take into account properly the Pauli exclusion principle. A way to overcome such a problem has been proposed in [89, 25]. By using this approach we performed some preliminary numerical simulations with different values of the Fermi energy (and as consequence the electron density) in a range where the unipolar description is justified. Bipolar simulations require major improvements into the scheme and will be performed in the future.

As appears from the plots, the electron-electron scattering makes the mean velocity lower and the relative importance of the electron-electron interaction reduces by increasing the Fermi energy. The latter has a simple explanation: at high density the Pauli principle considerably reduces the frequency of the electron-electron scatterings.

Similarly, the average energy per electron has a lower value when the electron-electron scattering is included.

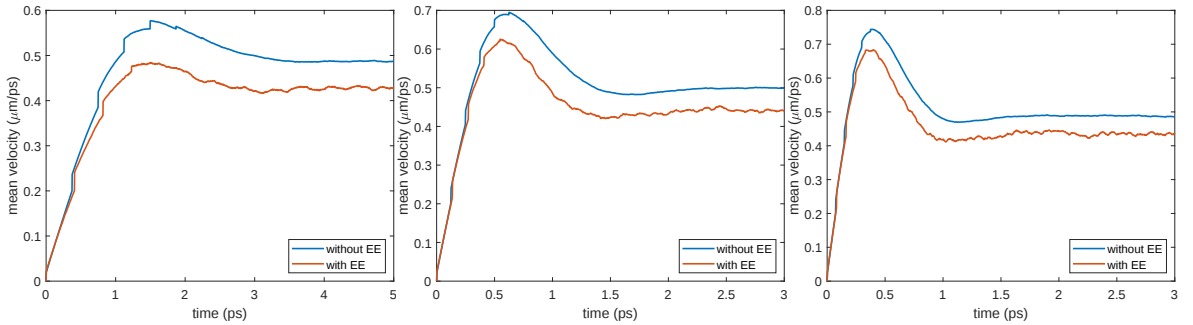


FIGURE 7.1: Mean velocity versus time at Fermi level 0.15 eV and electric field 1kV/cm, 3kV/cm, 5kV/cm.

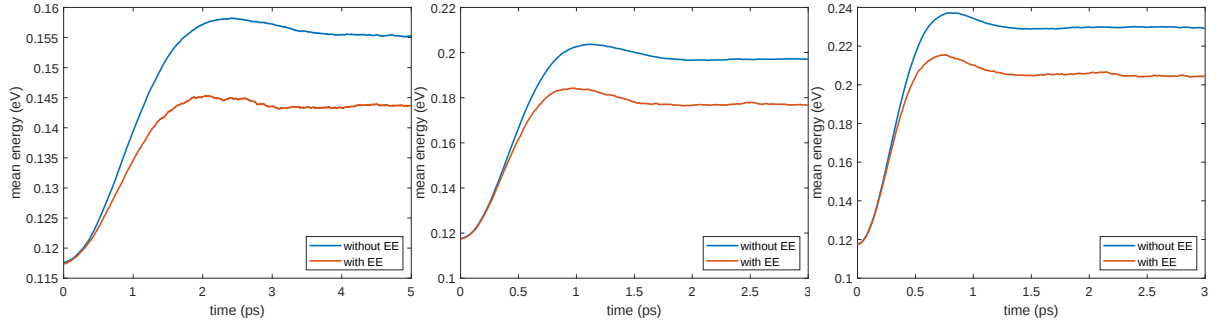


FIGURE 7.2: Mean energy versus time at Fermi level 0.15 eV and electric field 1kV/cm, 3kV/cm, 5kV/cm.

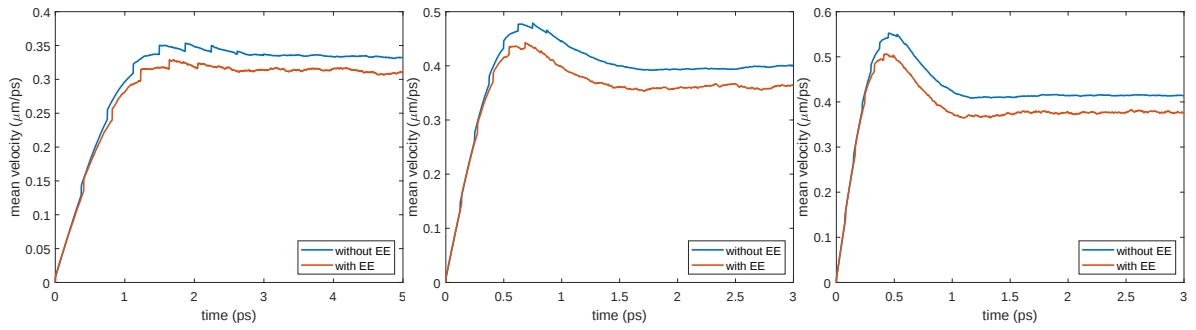


FIGURE 7.3: Mean velocity versus time at Fermi level 0.25 eV and electric field 1kV/cm, 3kV/cm, 5kV/cm.

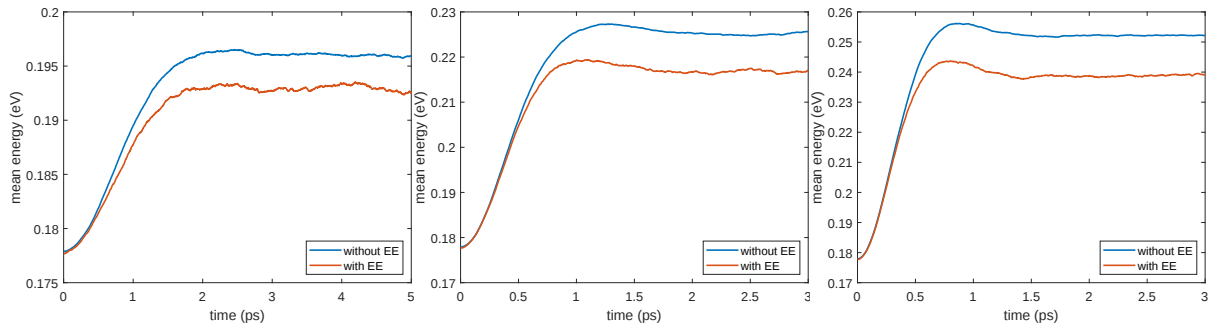


FIGURE 7.4: Mean energy versus time at Fermi level 0.25 eV and electric field 1kV/cm, 3kV/cm, 5kV/cm.

7.2 Discontinuous Galerkin approach for the simulation of charge transport in graphene in the non homogeneous case

In the last years an increasing interest has been devoted to graphene field effect transistors (GFETs) as potential candidates for high-speed analog electronics, where transistor current gain is more important than ratio current ON/current OFF [70]. Several types of GFETs have been considered in the literature [95]: top-gated graphene based transistors, obtained synthesizing graphene on silicon dioxide wafer, and double gate GFETs. The current-voltage curves present a behaviour different from that of devices made of classical semiconductors, like Si or GaAs, because of the zero gap in monolayer graphene. The current is no longer a monotone function of the gate voltage but there exists an inversion gate voltage corresponding to which the type of majority carriers changes. This introduces a certain degree of uncertainty in the determination of the current-off regime which requires a rather well tuning of the gate-source voltage. Usually the considered type of devices are investigated by adopting reduced one dimensional models with some averaging procedure [47, 103] and by describing the charge transport with drift-diffusion models, e.g. that given in [33]. Here we solve directly the semiclassical Boltzmann equation for electrons in graphene by using a discontinuous Galerkin (DG) method. If we consider for simplicity the unipolar and single valley case, the semiclassical Boltzmann equation for electrons in graphene reads

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{x}} f - \frac{q}{\hbar} \mathbf{E} \cdot \nabla_{\mathbf{k}} f = \mathcal{C}[f], \quad (7.1)$$

where the distribution function $f = f(t, \mathbf{x}, \mathbf{k})$, for any t , is defined on $D \times \mathbb{R}^2$ with $D \subset \mathbb{R}^3$. $\mathbf{E}$ is the electric field while the group velocity is given by $\mathbf{v}(\mathbf{k}) = \frac{1}{\hbar} \nabla_{\mathbf{k}} \varepsilon$, being $\varepsilon(\mathbf{k}) = \hbar v_F |\mathbf{k}|$ the dispersion relation in graphene around the Dirac points in the Brillouin zone. The collision term is given by

$$\begin{aligned} \mathcal{C}[f](t, \mathbf{x}, \mathbf{k}) = & \int S(\mathbf{k}', \mathbf{k}) f(t, \mathbf{x}, \mathbf{k}') (1 - f(t, \mathbf{x}, \mathbf{k})) d\mathbf{k}' \\ & - \int S(\mathbf{k}, \mathbf{k}') f(t, \mathbf{x}, \mathbf{k}) (1 - f(t, \mathbf{x}, \mathbf{k}')) d\mathbf{k}', \end{aligned}$$

where the total transition rate $S(\mathbf{k}, \mathbf{k}')$ is given by the sum of the contributions of the several types of scatterings

$$S(\mathbf{k}', \mathbf{k}) = \sum_{\nu} \left| G^{(\nu)}(\mathbf{k}', \mathbf{k}) \right|^2 \left[\left(n_{\mathbf{q}}^{(\nu)} + 1 \right) \delta \left(\varepsilon(\mathbf{k}) - \varepsilon(\mathbf{k}') + \hbar \omega_{\mathbf{q}}^{(\nu)} \right) + n_{\mathbf{q}}^{(\nu)} \delta \left(\varepsilon(\mathbf{k}) - \varepsilon(\mathbf{k}') - \hbar \omega_{\mathbf{q}}^{(\nu)} \right) \right].$$

The index ν labels the ν th phonon mode, $\left| G_{s',s}^{(\nu)}(\mathbf{k}', \mathbf{k}) \right|$ is the matrix element, which describes the scattering mechanism, due to phonons of type ν , between electrons belonging to the band s' and electrons belonging to the band s . The symbol δ denotes the Dirac distribution function, $\omega_{\mathbf{q}}^{(\nu)}$ is the ν th phonon frequency, $n_{\mathbf{q}}^{(\nu)} = \frac{1}{e^{\hbar \omega_{\mathbf{q}}^{(\nu)} / k_B T} - 1}$ is the Bose-Einstein distribution for the phonon of type ν , k_B is the Boltzmann constant and T is the graphene lattice temperature which will be kept constant.

For several geometries of graphene field effect transistors the charge flow is along a one dimension. If we assume that the motion is along the x -axis, then the Boltzmann equation writes

$$\frac{\partial f}{\partial t} + v_F \frac{k_x}{|\mathbf{k}|} \frac{\partial f}{\partial x} - \frac{q}{\hbar} E_x \frac{\partial f}{\partial k_x} = \mathcal{C}[f], \quad (7.2)$$

where $E_x = E_x(t, x)$ and $f(t, \cdot, \cdot)$ is now defined on $[0, L] \times \mathbb{R}^2$.

We adopt a DG method for solving Eq. (7.2), augmented with suitable initial conditions and boundary data. By requiring that $f(t, \mathbf{x}, \mathbf{k})$ tends to zero as $\mathbf{k} \mapsto \infty$, we assume that $f(t, x, \cdot) \approx 0$ on $\mathbb{R}^2 \setminus \Omega$ where $\Omega \subset \mathbb{R}^2$ is a compact set and introduce the decomposition

$$C_{i\alpha} = I_i \times B_{\alpha} =]x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}[\times B_{\alpha}, \quad i = 1, \dots, M, \quad \alpha = 1, \dots, N, \quad (7.3)$$

being $B_{\alpha} \subset \Omega$ open disjoint sets, such that $[0, L] \times \Omega = \bigcup_{i=1}^M \bigcup_{\alpha=1}^N \overline{C_{i\alpha}}$.

In each cell $C_{i\alpha}$ we approximate the solution with an element of the finite dimensional functional space spanned by $\varphi_1(t, x) = 1$, $\varphi_2(t, x) = \frac{x - x_i}{|I_i|}$, $\forall x \in I_i$, $\forall t > 0$, $\forall \mathbf{k} \in B_{\alpha}$, that is in each cell $C_{i\alpha}$ $f(t, x, \mathbf{k}) \approx a_{i\alpha}(t) + b_{i\alpha}(t) \frac{x - x_i}{|I_i|}$.

In order to get a system of evolution equations for the coefficients $a_{i\alpha}(t)$ and $b_{i\alpha}(t)$, we test the equation (7.2) against the two basis elements φ_1 e φ_2 . The main issue arises in the treatment of the numerical flux at the interface between adjacent cells. As already done for the homogenous case [89, 25, 63], a uniform non oscillatory (UNO) reconstruction is used.

7.2.1 Numerical simulations

As test case we simulate the charge transport in the GFET represented in Figure 7.5. The length is 40 nm, the total height is 21 nm. The graphene is placed between two layers of oxide (SiO_2), having width 10 nm each one. At the bottom and on the top there are two metallic gate contacts with applied voltages, V_{Gd} and V_{Gu} respectively. The source and drain contacts, each one long 10 nm, are placed over the graphene layer with applied voltages V_S and V_D . As discussed in [82], the electric potential,

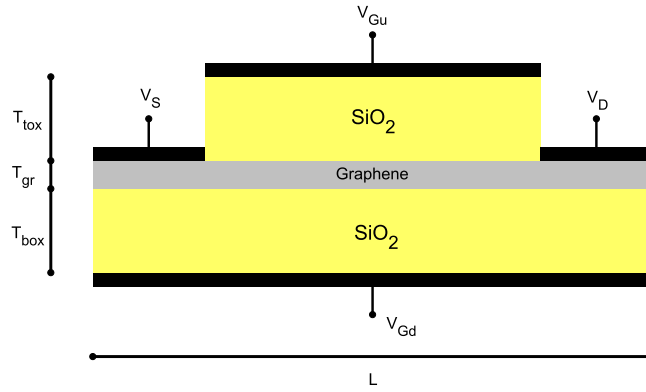


FIGURE 7.5: Schematic representation of a GFET.

see Figure 7.6, is obtained by a special treatment of the Poisson equation in which the charge in the graphene sheet is distributed in a strip having a thickness of 1 nm, and, at the contacts, it is determined by employing the peculiar relations between the electric potential and the carrier density in terms of a work function (see [53]). Moreover, we take, at the metallic contacts, voltages which are high enough to neglect the motion of holes.

For the preliminary results a time-independent electric field, deduced from the electric potential plotted in Figure 7.6, is considered. Such a potential has been obtained by simulating the charge transport with a drift-diffusion model [82]. In Figures 7.7 we report the steady solution obtained after 1 ps by numerically solving the Boltzmann equation with the DG method. In the present simulations the scatterings with the impurities and the optical phonons of the substrate have been neglected but they can be easily included. A major issue is the setting of the boundary conditions at source and drain because, at variance with standard semiconductor devices, there is no doping and the contact is directly over the graphene. We model the contacts as charge reservoirs. Inside them we assume that the electron distribution is a Fermi Dirac at a room temperature. Therefore the mean values of the electron velocity is zero inside the contacts even if it is nonzero in the channel. As a consequence a boundary layer in the current appears at the interfaces contact/graphene which is plotted in Fig. 7.7 (left) as a dashed line.

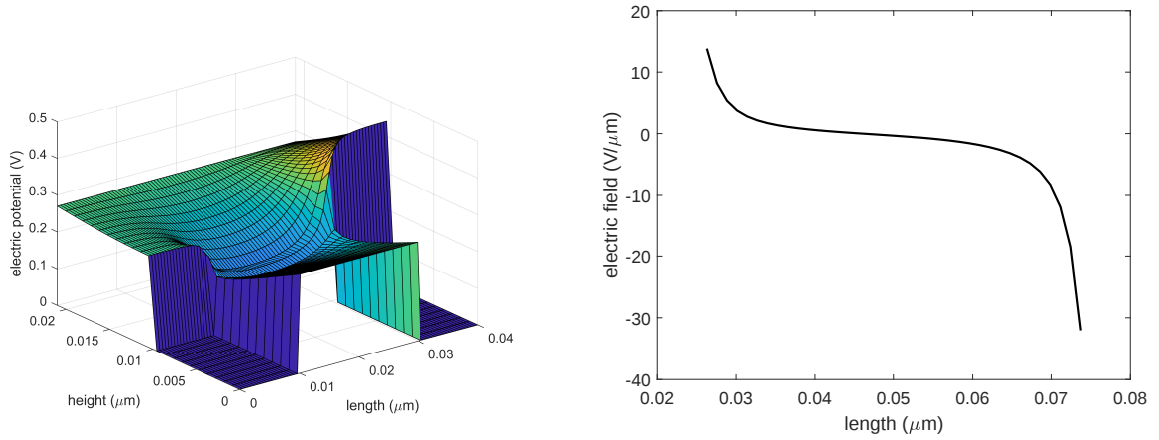


FIGURE 7.6: Electric potential (left) and electric field (right) along the graphene sheet in the case of gate voltage 0.02 V and bias 0.2 V. The work function at source and drain is set 0.25 eV.

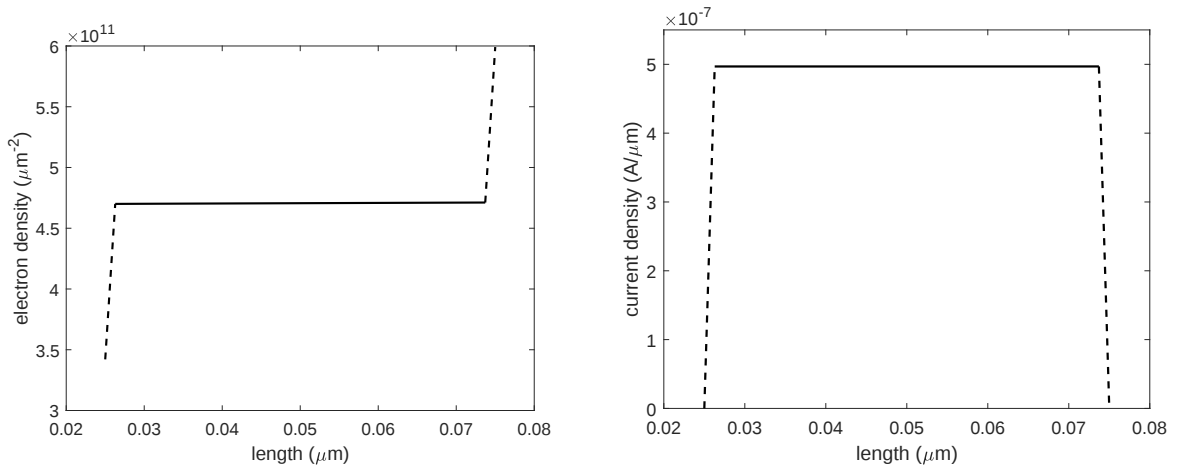


FIGURE 7.7: Steady density (left) and current (right). The dashed parts represent the boundary layers arising at the contact/graphene interfaces.

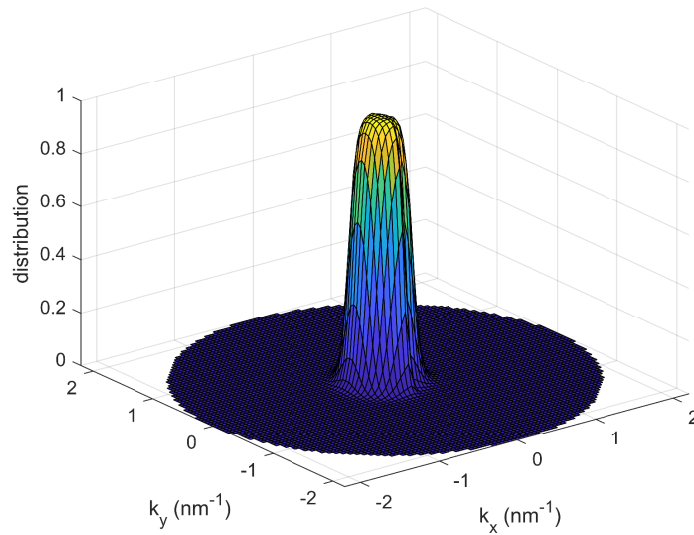


FIGURE 7.8: Steady electron distribution at the middle of the channel.

Conclusions

The topic of modeling and simulation of charge transport in graphene has been tackled from various points of view. In monolayer graphene the bipolar charge transport has been simulated by a numerical deterministic approach, based on a discontinuous Galerkin (DG) method [63, 27]. The semiclassical Boltzmann equations have been solved numerically. Both the conduction and valence bands have been included and the interband scatterings have been taken into account. The importance of the interband scatterings has been accurately evaluated for several values of the Fermi energy. Both suspended graphene and graphene on an h-BN substrate have been considered and numerical results have been discussed in Chapter 3. The interband interaction is relevant for values of the Fermi energy around zero eV and it becomes negligible by increasing the absolute value of the Fermi energy. For the suspended case if ε_F is greater than 0.2 eV, the interband effects can be eliminated without any significant consequence in the simulations. If an h-BN substrate is included this value reduces to 0.1 eV. Moreover the time at which the steady state is reached depends on the interband interaction and on the presence of a substrate.

In Chapter 4 new mobility models for charge transport in graphene have been obtained by a fitting procedure based on data derived from the numerical solutions of the Boltzmann transport equations by means of the DG approach [81]. Both the cases of suspended graphene and graphene on substrate have been considered. Comparisons with other models present in the literature show a considerable improvement. An analysis of the high-field mobility has been performed for graphene on a substrate by the new DSMC approach of ref. [89], which properly takes into account the Pauli exclusion principle. Moreover, also the random distribution of the depth of the impurities implanted in the oxide has been taken into account and described with several theoretical probability distributions. Section 4.4 has been devoted to the simulation of a graphene based field effect transistor, proposing a full coupled drift-diffusion-Poisson simulation based on finite differences schemes. At first instance the model has been developed adopting the mobility model of ref. [33] and numerical results have been shown in [82]. Such a device suffers from the difficult determination of the current-off state because, due to the capacitance effects of graphene, the holes population becomes dominant and led to an increasing total current by decreasing the gate voltages. A more detailed analysis has been presented in [79] where the new mobility models including

the effects of a substrate, introduced in the first part of the chapter, have been adopted. The results confirm the limited range of gate-source voltages for the current-off state.

As possible further improvements, which are in part under investigation could be the inclusion of thermal effects, along the results obtained for suspended monolayer graphene [26, 30, 29], and the introduction of quantum corrections, as in [72, 7, 75, 59]. Two forthcoming researches have been discussed in Chapter 7 regarding the simulation of the electron-electron interaction by a DSMC approach and the numerical solutions of the Boltzmann transport equation in non homogeneous case by a DG approach.

In Chapter 5 a study on quantum-drift-diffusion model have been outlined in two dimensional case, based on [9, 10], with the idea to be able to describe the Klein tunneling effect in graphene. Numerical simulations have been performed for the device of ref. [108]. We have found the presence of oscillations in the conductance and their behavior in terms of period looks qualitatively similar to the experimental data of [108]. A further improvement of the agreement requires a more physically accurate model. A possible development will be the mobility models and the coupling with the Poisson equation.

In Chapter 6 we have explored the possibility to define and numerically solve an optimal control problem involving the semiclassical Boltzmann equation for charge transport in graphene. We proposed to minimize the discrepancy of the electron distribution function with respect to a prescribed probability density to reach at final time, to confine the electron wave vectors in average during the evolution, keeping the electric field the minimum in modulus. A system of integro-differential partial differential equations have been obtained and a discretization based on a DG approach has been proposed. Numerical results are postponed to forthcoming papers.

To conclude we remark that the studies performed during the three years of PhD have led to several papers of which four published [24, 27, 63, 81], one in press [82] and five submitted or in preprint version [8, 11, 28, 79, 80].

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