The free flight step analysis in the Monte Carlo Method. Test case: charge transport in graphene.

Marco Coco*

Abstract

Monte Carlo methods are now a definitively well established methods for studying the transport of charges in semiconductors. A lot of drawbacks are however present about the correct reconstruction of the distribution function, which has to be bounded between 0 and 1. The standard Ensemble Monte Carlo method is not able to properly include the Pauli exclusion principle and the numerical distribution functions exceed the maximum value. A lot of attempts were made to solve the problem and recently a new DSMC scheme has been developed to overcome the problem. All the improvements are generally based on some approximations or computational techniques involving the distribution function and the scattering terms. Only an attempt was devoted to opportunely change the formulation of the free flight step but there is still a lack in the literature regarding a both theoretical and computational analysis of corrected Monte Carlo methods based on the free flights. In this paper we would like to fulfill such a gap by analyzing deeper the role of the free flight step into a Monte Carlo simulation, its physical properties and the conditions that allow us to preserve the physical consistency of the method.

Keywords Monte Carlo Method, free flight, Pauli exclusion principle

*Dipartimento di Ingegneria Industriale e Scienze Matematiche, Università Politecnica delle Marche, via Brecce Bianche, 12, 60131 Ancona, Italy (m.coco@univpm.it),
1 Introduction

The Monte Carlo method is certainly one of the most intellectually stimulating mathematical ones for its peculiar nature to be able to solve deterministic problems by using stochastic procedures. For this reason, it is really useful for a direct description of problems typically formulated in a macroscopic and/or kinetic way, in any case respect to a population or a control volume. The mathematical description of transport problems at a kinetic level is always based on a distribution function that assigns to each particles a measure of probability and then the itself distribution function is studied. The Monte Carlo method makes possible to reach this result but at the same time to look to each “representative” particle individually. For this peculiar property the MC method has been started to be theorized and used to simulate problems involving a great number of particles. One of the fields where it is definitely a standard method is that of the charge transport in semiconductors. Starting from the pioneering works of Bosi and Jacoboni [1], Jacoboni and Reggiani [2] for one particle, Lugli and Ferry developed a MC method for the charge transport in semiconductors based on the description of an entire population of particles [3], the so called Ensemble Monte Carlo Method (EMC). The simulations performed by using this global approach are often called Direct Simulations Monte Carlo (DSMC), which emphasizes the direct-to-particle property of Monte Carlo.

The semiclassical approach is used; each particle is a wave-packet, with its own group velocity, but so picked to be treated as a particle. The involved equations are the Boltzmann ones for the charge distribution function, that assigns to each particle the probability to be found in a given volume element. In the Boltzmann equations there is the balance between the streaming and drift terms and the contribution of the collision operator. This last one describes the interactions between the particles and between the particles and the crystal lattice. In an analog way, the main steps of the Monte Carlo procedure are the free flight of the particles, when the streaming term and the drift one due to the applied fields are solved, interrupted by collision events; both the steps
are based on the generation of random numbers (see the following section for more details). The main difficulties arise from the collision operator because for an its complete description one has to know all the initial states of the particles but also the final states, so it has to integrate with respect to all the possible final states. This is a hard task both from an analytical point of view and from a computational one; it would make the computation practically impossible. In [3], a rejection technique has been proposed to overcome the problem, so the particle dynamics is completely solved a part the availability of the final states and in a following step the final state is checked by means of the rejection technique; also this step is based on the use of random numbers. The importance of the availability of the final states is physically due to the Pauli exclusion principle for the electrons and mathematically to the boundedness of the distribution function between 0 and 1.

The rejection technique started to fail when the degenerate gases, with very high electron density, were considered; with the standard EMC one could be calculate acceptable mean values for the energy and the velocity of the particles but the distribution function is not correctly reconstructed, exceeding the maximum value 1. This is of fundamental importance in high densities semiconductors because the distribution function in turn enters the collision operator and affects the evolution of the scattering events.

A lot of attempts can be found in the literature to overcome such a problem. The standard ones are based on the introduction of ad hoc scattering out terms to force the distribution function to be less than 1 [4, 5] or on ad hoc approximation of the distribution function of the final states [6, 7]. They improved the simulation results but did not solve the basic problem of a correct reconstruction of the distribution function. Recently in [8], by means of an hybrid approach and a splitting between the free flight step and the scattering one, a new DSMC procedure has been developed with a correct inclusion of the Pauli exclusion principle without any unphysical ad hoc approximations.

All the ways to solve the previous problem have involved the scattering term and the related distribution functions. A solution to include the Pauli exclusion
principle and then to correctly calculate the distribution functions by acting not on the collision operator but on the free flight step was proposed in [9]; the rejection technique proposed in [3] and that would ensure the respect of Pauli’s principle is applied not only at the end of the scattering but also at the end of the free flight, i.e. the position of the particle after the free flight has occurred is checked before it is allowed to scatter. This approach deserves to be mentioned and will be the subject of this paper because it leads to very significant both computational and theoretical considerations. Indeed, a considerable literature about the treatment of the collisional part is available, but it is not the same about the role of the free flight in the Monte Carlo method. It is a fundamental question that should be answered whether free flight in the Monte Carlo method for degenerate semiconductors follows the laws of classical physics or quantum mechanics. Nevertheless, the procedure in [9] is highly cited, both in support and not, see [4, 5, 7, 23, 24] for example, but always from only a computational point of view; it can not be found, at our knowledge, a satisfactory theoretical analysis of such an approach, and up to now there is a lot of conflicting opinions, but almost only opinions, about the treatment and the physical nature of the free flight step.

The aim of the paper is to fill this gap in an as exhaustive and conclusive as possible way. We solve the charge transport in monolayer suspended graphene as a test case by using the standard EMC in [3] and the new DSMC in [8], that are by now well established in the semiconductors fields and cross-validated with deterministic solutions, for example those based on the discontinuous Galerkin method [8, 10, 11] or on WENO schemes [12]. Then we compare the previous results with those obtained by adopting the approach in [9], and an analysis both theoretical and computational will be done. The results obtained by using the EMC and the new DSMC are already showed in [8] and allows us to quantify the correctness of the method proposed in [9]. Besides, graphene is a material with a very high electron density and the degeneracy effects cannot be neglected, so it is a useful choice as test case.

The paper is organized as follows. In section 2 a summary of the Monte
Carlo methods used in the paper is given, in section 3 the semiclassical mathematical model for graphene is presented, in sections 4, 5 the results are showed and then discussed.

2 Monte Carlo procedures

2.1 The standard EMC scheme

We simulate independently the dynamics of $N$ particles described according to a distribution function $f$. Each particle is a super particle and represents a certain number of real particles $N^*$, with a statistical weight equal to the ratio $N^*/N$. Given an initial condition for $f$, we define a time window $\Delta t$ and follow the motion of each particle within $\Delta t$. The motion is a free flight determined by the semiclassical equations of motion and it is interrupted by collision events between the particle with other particles or between the particle and the crystal lattice. The main steps of EMC procedure are

- the choice of the free flight duration $dt$
- the choice of the type of scattering
- the calculation of the energy and of the momentum of the particle after the collision
- the use of the rejection technique to check the availability of the final state
- the updating of the values of energy, momentum of the particle and of the distribution function $f$ if the final state is available, otherwise the scattering is rejected and it didn’t happen
- a new free flight time $dt$ is generated and the procedure is repeated until $\Delta t$ is reached
- at $\Delta t$ the mean energy and the velocity of the particles are calculated and recorded
This procedure is followed independently for each particle, that in turn are synchronized, i.e. $dt$ is equal for each particle. There are good results about the mean values thanks to the great number law, but the condition $0 \leq f \leq 1$ is not respected by using this scheme.

2.2 The new DSMC scheme

As stated in [8] the main steps are:

- choice of the free flight duration $dt$
- a rigid translation of the distribution function $f$ as a whole, i.e. all the particle experience the same free flight without scattering events; the energy and momentum of all particles are updated. In this way the occupation number of each cell of the computational grid does not change
- the time is frozen and the collision events involving each particle are considered; for each particle the availability of the final state is checked by means of the rejection technique; if it is available the energy, momentum and distribution function are updated, otherwise nothing happens
- the procedure is repeated until $\Delta t$ is reached, when the mean values of the energy and momentum are calculated and recorded

2.3 The free flight-based Monte Carlo scheme

It is the same of the standard EMC with the only difference that the Pauli exclusion principle is applied also at the end of each free flight of each particle and not only at the end of a scattering events [9]. The main steps are:

- the choice of the free flight duration $dt$
- introduction of a rejection technique to check the availability of the state reached at the end of the free flight; if it is available the particle dynamics continues, otherwise nothing happens and the particle returns to the initial state before the free flight
• the choice of the type of scattering

• the calculation of the energy and of the momentum of the particle after the collision

• the use of the rejection technique to check the availability of the final state

• the updating of the values of energy, momentum of the particle and of the distribution function \( f \) if the final state is available, otherwise the scattering is rejected and it didn’t happen

• a new free flight time \( dt \) is generated and the procedure is repeated until \( \Delta t \) is reached

• at \( \Delta t \) the mean energy and the velocity of the particles are calculated and recorded

3 The kinetic semiclassical mathematical model

The electron energy in graphene depends on a two dimensional wave-vector \( k \) belonging to a bi-dimensional Brillouin zone \( B \) which has a hexagonal shape.

Most of the electrons are in the valleys around the vertices of the Brillouin zone, called Dirac points or \( K \) and \( K' \) points. Usually the \( K \) and \( K' \) valleys are treated as a single equivalent one.

In a semiclassical kinetic setting, the charge transport in graphene is described by four Boltzmann equations, one for electrons in the valence band (\( \pi \)) and one for electrons in the conduction band (\( \pi^* \)), that in turn can belong to the \( K \) or \( K' \) valley,

\[
\frac{\partial f_{\ell,s}(t,x,k)}{\partial t} + v_{\ell,s} \cdot \nabla_x f_{\ell,s}(t,x,k) - \frac{e}{\hbar} \mathbf{E} \cdot \nabla_k f_{\ell,s}(t,x,k) = \left. \frac{df_{\ell,s}}{dt}(t,x,k) \right|_{e^{-ph}}
\]

where \( f_{\ell,s}(t,x,k) \) represents the distribution function of charge carriers, in the band \( \pi \) or \( \pi^* \) (\( s = -1 \) or \( s = 1 \)) and valley \( \ell \) (\( K \) or \( K' \)), at position \( x \), time \( t \), and with wave-vector \( k \). We denote by \( \nabla_x \) and \( \nabla_k \) the gradients with respect
to the position and the wave-vector, respectively. The group velocity \( v_{\ell,s} \) is related to the band energy \( \varepsilon_{\ell,s} \) by

\[
v_{\ell,s} = \frac{1}{\hbar} \nabla_{\mathbf{k}} \varepsilon_{\ell,s}.
\]

With a very good approximation \[13\], a linear dispersion relation holds for the band energies \( \varepsilon_{\ell,s} \) around the equivalent Dirac points, so that

\[
\varepsilon_{\ell,s} = s \hbar v_F |\mathbf{k} - \mathbf{k}_\ell|,
\]

where \( v_F \) is the (constant) Fermi velocity, \( \hbar \) the Planck constant divided by \( 2\pi \), and \( \mathbf{k}_\ell \) is the position of the Dirac point \( \ell \). We will assume the (2) as dispersion relation because for the electric fields usually considered in the applications the charge transport involves almost exclusively the electrons around the \( K \) points.

The elementary (positive) charge is denoted by \( e \), and \( \mathbf{E} \) is the electric field, here considered as an external field. The right hand side of Eqs. (1) is the collision term representing the interactions of electrons with acoustic, optical and \( K \) phonons. Acoustic phonon scattering is intra-valley and intra-band and can be longitudinal (\( LA \)) or transversal (\( TA \)). Optical phonon scattering is intra-valley and can be longitudinal (\( LO \)) and transversal (\( TO \)); it can be intra-band, leaving the electrons in the same band, or inter-band, pushing the electrons from the initial band toward another one. Scattering with phonons of \( K \)-type pushes electrons from a valley to a nearby one (inter-valley scattering). The general form of the collision term can be written as (see \[13\] \[12\] for more details)

\[
\left. \frac{df_{\ell,s}(t,\mathbf{x},\mathbf{k})}{dt} \right|_{\mathit{e-ph}} = \sum_{\ell',s'} \left[ \int_{\mathcal{B}} S_{\ell',s',\ell,s}(\mathbf{k}',\mathbf{k}) f_{\ell',s'}(t,\mathbf{x},\mathbf{k}') (1 - f_{\ell,s}(t,\mathbf{x},\mathbf{k})) d\mathbf{k}' \right. \\
\left. - \int_{\mathcal{B}} S_{\ell,s,\ell',s}(\mathbf{k},\mathbf{k}') f_{\ell,s}(t,\mathbf{x},\mathbf{k}) (1 - f_{\ell',s'}(t,\mathbf{x},\mathbf{k}')) d\mathbf{k}' \right],
\]

where the total transition rate \( S_{\ell',s',\ell,s}(\mathbf{k}',\mathbf{k}) \) is given by the sum of the contributions of the several types of scatterings described above

\[
S_{\ell',s',\ell,s}(\mathbf{k}',\mathbf{k}) = \sum_A \left| G^{(A)}_{\ell',s',\ell,s}(\mathbf{k}',\mathbf{k}) \right|^2 \left[ (g_A^- + 1) \delta(\varepsilon_{\ell,s}(\mathbf{k}) - \varepsilon_{\ell',s'}(\mathbf{k}') + \hbar \omega_A) \\
+ g_A^+ \delta(\varepsilon_{\ell,s}(\mathbf{k}) - \varepsilon_{\ell',s'}(\mathbf{k}') - \hbar \omega_A) \right].
\]
The index \( A \) labels the \( A \)th phonon mode. The \( G^{(A)}_{\ell',s',\ell,s}(k',k) \)'s are the electron-phonon coupling matrix elements, which describe the interaction mechanism of an electron with an \( A \)th phonon, from the state of wave-vector \( k' \) belonging to the valley \( \ell' \) and band \( s' \) to the state of wave-vector \( k \) belonging to the valley \( \ell \) and band \( s \). The symbol \( \delta \) denotes the Dirac distribution, \( \omega_A \) is the \( A \)th phonon frequency, \( g_A(q) \) is the phonon distribution for the \( A \)-type phonons with \( q \) the phonon wave-vector belonging to \( B \). In (3), \( g_A^\pm = g_A(q^\pm) \), where \( q^\pm = \pm(k' - k) \), stemming from the momentum conservation.

For both longitudinal and transversal acoustic phonons, we consider the elastic approximation according to which the transition rate reads\[14\]
\[
\frac{1}{(2\pi)^2} \frac{\pi D_{ac}^2 k_B T}{2\hbar \sigma_m v_s^2} (1 + \cos \theta_{k,k' - k}) \delta(\varepsilon(k') - \varepsilon(k)), \quad s = LA, TA
\]
where \( D_{ac} \) is the acoustic phonon coupling constant, also called acoustic phonon deformation potential, \( \sigma_m \) is the graphene areal density, and \( \theta_{k,k'} \) is the convex angle between \( k \) and \( k' \). The values of the parameters used in the present paper are indicated in Table 1.

The electron-phonon coupling matrix elements of the longitudinal optical (LO), the transversal optical (TO) and the \( K \) phonons are (see for example [12])
\[
\begin{align*}
|G^{(LO)}(k',k)|^2 &= \frac{1}{(2\pi)^2} \frac{\pi D_{O}^2}{\sigma_m \omega_{O}} (1 - \cos(\theta_{k,k' - k} + \theta_{k',k' - k})) \\
|G^{(TO)}(k',k)|^2 &= \frac{1}{(2\pi)^2} \frac{\pi D_{O}^2}{\sigma_m \omega_{O}} (1 + \cos(\theta_{k,k' - k} + \theta_{k',k' - k})) \\
|G^{(K)}(k',k)|^2 &= \frac{1}{(2\pi)^2} \frac{2\pi D_{K}^2}{\sigma_m \omega_{K}} (1 - \cos \theta_{k,k'})
\end{align*}
\]
where \( D_{O} \) is the optical phonon coupling constant, \( \omega_{O} \) the optical phonon frequency, \( D_{K} \) is the \( K \) phonon coupling constant and \( \omega_{K} \) the \( K \) phonon frequency.

The angles \( \theta_{k,k' - k} \) and \( \theta_{k',k' - k} \) denote the convex angles between \( k \) and \( k' - k \) and between \( k' \) and \( k' - k \), respectively.

In our numerical simulations of monolayer graphene, the parameters proposed in [15, 16] have been adopted. They are reported in Table 1. In the sequel we will consider only cases of high values of the Fermi energy, which are
Table 1: Physical parameters for the scattering rates.

| Parameter | Value |
|-----------|-------|
| $\sigma_m$ | $7.6 \times 10^{-8}$ g/cm$^2$ |
| $v_F$     | $10^6$ m/s |
| $v_{LA}$  | $2.13 \times 10^4$ m/s |
| $v_{TA}$  | $1.36 \times 10^4$ m/s |
| $D_{ac}$  | 6.8 eV |
| $\hbar \omega_{LO}$ | 164.6 meV |
| $\hbar \omega_{TO}$ | 164.6 meV |
| $D_O$     | $10^9$ eV/cm |
| $\hbar \omega_K$ | 124 meV |
| $D_K$     | $3.5 \times 10^8$ eV/cm |

equivalent for conventional semiconductors to a n-type doping. Under such a condition the dynamics of the electrons belonging to the valence band can be neglected. In order to simplify the notation the indices $s$ and $\ell$ will be omitted.

Regarding the optical and $K$ phonons we will assume the Einstein approximation: $\hbar \omega_\eta$ is constant, $\eta = LO, TO, K$. Instead, for the in plane acoustic phonons the Debye approximation will be assumed, $\hbar \omega_s = \hbar v_s |q|$, $s = LA, TA$, and in this case for the analytical calculations the Brillouin zone can be consistently extended to $\mathbb{R}^2$.

We remark that the $K$ phonons do not constitute an actual physical phonon branch. Their name is due to the fact that their wave-vectors are close to the $K$ or $K'$ point [13]. They belong to the optical branches and induce intervalley scatterings. This justifies the use of the Einstein approximation for them.

The scattering rate of the $A$th type of scattering is defined as

$$\Gamma_A(k) = \int S_A(k,k') \, dk'.$$

For the acoustic phonon scattering we get

$$\Gamma_{ac}(\varepsilon) = \frac{D_{ac}^2 k_B T}{4 \hbar^3 v_p^2 \sigma_m v_p^2} \varepsilon.$$

and for the longitudinal and transversal optical phonon, respectively,
Figure 1: Scattering rates evaluated with the Bose-Einstein equilibrium distributions for phonons at the temperature of 300 K.

\[
\Gamma_{LO,TO}(\varepsilon) = \frac{D_O^2}{4\pi\sigma_m \omega_O h^2 v_F} \left[ (\varepsilon - \hbar \omega_O)(g_{LO,TO} + 1)H(\varepsilon - \hbar \omega_O)(2\pi - \Lambda^{-}(\varepsilon)) \\
+ (\varepsilon + \hbar \omega_O)g_{LO,TO}(2\pi + \Lambda^{+}(\varepsilon)) \right].
\]

The upper and the lower signs refer to the LO and TO phonons, respectively. Here \( H \) is the Heaviside function and

\[
\Lambda^\pm(\varepsilon) = \frac{1}{\varepsilon(\varepsilon \pm \hbar \omega_O)} \int_0^{2\pi} \frac{(2\varepsilon^2 + \hbar^2 \omega_O^2 \pm 2\hbar \omega_O \varepsilon) \cos \theta'' - 2\varepsilon(\varepsilon \pm \hbar \omega_O) \cos \theta''}{(2\varepsilon^2 + \hbar^2 \omega_O^2 \pm 2\hbar \omega_O \varepsilon - 2\varepsilon(\varepsilon \pm \hbar \omega_O) \cos \theta'')} d\theta''
\]

\[
= -\frac{\pi}{\varepsilon(\varepsilon \pm \hbar \omega_O)} \left( 2\varepsilon^2 + \hbar^2 \omega_O^2 \pm 2\hbar \omega_O \varepsilon - \hbar \omega_O|2\varepsilon \pm \hbar \omega_O| \right) .
\]

Similarly, the expression of the scattering rate for the \( K \) phonon scattering reads

\[
\Gamma_K(\varepsilon) = \frac{D_K^2}{\sigma_m \omega_K h^2 v_F^2} \left[ (\varepsilon - \hbar \omega_K)(g_K + 1)H(\varepsilon - \hbar \omega_K) + (\varepsilon + \hbar \omega_K)g_K \right].
\]

In Fig. 1 the scattering rates for each type of phonons are shown.
4 Simulation results

The physical situation we simulate is that of a strip of graphene which is infinitely long in the transversal direction with respect to that of the electric field. This allows us to look for solutions which are not depending on space and to avoid any effect related to the boundary conditions.

We use \( n_p = 10^4 \) simulated particles, we set the time step equal to \( \Delta t = 2.5 \) fs and we consider the room temperature \( T = 300 \) K. For a homogeneous mono-layer graphene under a constant electric field \( \mathbf{E} \), the only significant components of the evolution equations are those parallel to the field and there is not dependence on the spatial variables. By choosing a reference frame in the plane of the graphene sheet with the x-axes parallel to \( \mathbf{E} \), the complete model consists of the following equations

\[
\frac{\partial f(t, k)}{\partial t} - \frac{e}{\hbar} E \frac{\partial f(t, k)}{\partial k_x} = \int S(k', k) f(t, k') (1 - f(t, k)) \, dk' \\
- \int S(k, k') f(t, k) (1 - f(t, k')) \, dk'.
\] (8)

As initial condition we take the Fermi-Dirac distribution

\[
f(0, k) = \frac{1}{1 + \exp\left(\frac{\varepsilon(k) - \varepsilon_F}{k_B T}\right)},
\] (9)

where \( \varepsilon_F \) is the Fermi energy, which is related to the initial charge density by

\[
\rho(0) = \frac{4}{(2 \pi)^2} \int f(0, k) \, dk.
\] (10)

In \([17]\) the factor 4 arises because we consider both the two states of spin and the degeneracy (equal to 2) of the valleys. Alternatively, one can consider the population of a single valley, and put the valley degeneracy equal to one and in \([17]\) take \( \rho(0)/2 \) as the electron density. Note that in the unipolar case \( \rho \) remains constant, \( \rho(t) = \rho(0) \), as a consequence of the charge conservation.

For the coupling of the phonon transport and for the convergence properties of the scheme with respect the number of particles and the values of \( \Delta t \), we refereee to \([17]\) \([18]\) and \([19]\), respectively.
The mean electron velocity and energy, $V$ and $E$, are defined as

$$V = \frac{4}{(2\pi)^2 \rho} \int f(t,k) v \, dk = \frac{4}{(2\pi)^2 \rho} \int f(t,k) \frac{1}{\hbar} \nabla_k \varepsilon \, dk,$$

(11)

and

$$E = \frac{4}{(2\pi)^2 \rho} \int f(t,k) \varepsilon \, dk.$$  

(12)

In this first part we show and discuss the results obtained by using the standard EMC and the new DSMC, then we focus on the analysis of the free-flight based Monte Carlo scheme.

In this paper the acoustic and optical phonon branches are split into the transversal and longitudinal ones. However, the inclusion of the anisotropy of the optical phonons does not produce perceptible difference in the numerical results. In Fig.s [2][4] the electrons distribution functions and their view along the electric field direction are shown for the simulations performed by using the standard EMC scheme and the new DSMC one, respectively. The standard EMC leads to a distribution function exceeding the maximum value equal to one and then to a manifest violation of the Pauli exclusion principle. Besides, the Pauli principle is respected in the new DSMC scheme; in this case, in Fig.s [2][4] the values of the wave-vector along the x-direction are due to the rigid translation of the computational grid along with the distribution function during the free flight step with a semi-lagrangian approach that reduces considerably the computational cost. Nevertheless, there is a good agreement between the mean values obtained by using both the two approaches (Fig. 4). This is can be explained by means of the large number law and the homogenization properties of the integrals underlying the calculation of the average values. Let be $n_\mu$, $\mu = LA, TA, LO, TO, K$, the number of the scatterings between electrons and each phonon branch, $n_{\mu-acce}$ and $n_{\mu-tot}$ the number of the scatterings accepted because of the availability of the final states and the total number of the scattering attempts, respectively; $r_\mu$ is the ratio between $n_{\mu-acce}$ and $n_{\mu-tot}$; $N_{acc} = \sum_\mu n_{\mu-acce}$ and $N_{tot} = \sum_\mu n_{\mu-tot}$. The values of these quantities are
reported in Table 2 both for the EMC and the DSMC case. We have almost the same values for both the schemes and this is a crucial evidence of the fact that both the two methods respect the dynamics of the problems and in particular, for our analysis, they respect the physical nature of the free flight between the collisions. In this sense, we could say that they simulate the same dynamics from a physical point of view, even if the EMC scheme suffers from a mathematical limit and it is not able to correctly reconstruct the distribution function.

It worth highlighting that the values of Table 2 are almost the same but the ones related to the EMC case are always higher because the availability of the final states is overestimated. This occurrence has not to be neglected when the distribution function has a crucial role in the physics of the material.

The temporal grid is divided into uniform steps $\Delta t$. A crucial, even if rarely
(a) Figure 3: View of the distribution functions along the x-axis after 5 ps for EMC, a), and new DSMC, b).  

|                | EMC | DSMC | EMC | DSMC | EMC | DSMC |
|----------------|-----|------|-----|------|-----|------|
| $n_{LA-acc}$   | 6027| 6027 | 11869| 11905| r_{LA} | 0.5078   | 0.5063   |
| $n_{TA-acc}$   | 15035| 14792| 29444| 29155| r_{TA} | 0.5106   | 0.5074   |
| $n_{em-acc}$   | 121242| 120122| 276531| 277485| r_{em} | 0.4384   | 0.4329   |
| $n_{LO-acc}$   | 686  | 632  | 930  | 898  | r_{ab} | 0.7376   | 0.7038   |
| $n_{em-acc}$   | 13126| 12837| 46382| 45953| r_{em} | 0.2830   | 0.2794   |
| $n_{ab-acc}$   | 74   | 85   | 119  | 156  | r_{ab} | 0.6218   | 0.5449   |
| $n_{em-acc}$   | 28707| 28740| 58811| 59254| r_{em} | 0.4881   | 0.4850   |
| $n_{ab-acc}$   | 541  | 571  | 772  | 849  | r_{ab} | 0.7008   | 0.6726   |
| $N_{acc}$      | 185438| 183806| 424858| 425655| r_{tot} | 0.4365   | 0.4318   |

Table 2: Number of accepted and total scatterings and their ratio in the EMC and new DSMC simulations after 5 ps, $\varepsilon_F = 0.6$ eV, $E = 20$ kV/cm.

Pointed out, aspect of Monte Carlo scheme is the treatment of the dynamics of the particle near the temporal grid edge, when, at time $t$, the random free flight duration $dt$ is such that $t + dt > \Delta t$. We cannot change $dt$ because it is equal for all the particles which must be synchronized. There are two choices: either to allow the particle to overcome the barrier $\Delta t$, to reach the time $t_{res} = t + dt - \Delta t$, and to wait until the other particles finished their dynamics in the previous time step, or to stop the particle at the edge with time $t = \Delta t$. This last one is that
Figure 4: Average energy and velocity in the EMC case, a), and in the new DSMC, b).
has been followed in our simulations with the EMC. This problem does not arise when the new DSMC is used because during the time evolution the particles are treated as a whole and only later they scatter with the crystal lattice. In Fig. 5-6, we compare the distribution functions and the mean energy and velocity of the EMC case obtained with the two approaches, respectively. The electron distribution function when residual time is allowed seems to respect the Pauli principle but this is fictitious because it is too much smeared in the wave-vector space; it reaches value even five times greater than those one of the correct Monte Carlo approach; indeed, the mean energy has values five times greater and it doesn’t reach a steady state value. The transient overshoot value of the velocity is three times greater and then it reaches the steady state value due to the homogenization of directions at long times. When the residual time over the temporal edge $\Delta t$ is allowed the dynamics is not well described; the particles are free to move avoiding a lot of interactions with the crystal lattice, as the Table 3 shows, where the number of the scatterings is reported and that is much lower than the other case; furthermore, when a scattering occurs is almost certainly accepted and the gas is no longer degenerate; in this way the particles reach positions far away from the origin of the reference frame in the Dirac point $K$ and they continue to increase their energy. This fact underlines the fundamental importance of the synchronization of the particles and it should be accurately taken into account also in the one-particle Monte Carlo and in those situations when the ergodicity is requested.

For the free-flight based Monte Carlo (FFMC) we take the same simulation parameters used above and as initial condition the Fermi-Dirac distribution of Eq. 10 and showed in Fig. 7(a). The electron distribution after 5 ps is shown in Fig.s 7(b)-c) and it is almost the same of the initial one. By using the Fermi-Dirac distribution, typical of a degenerate electron gas, the scheme is not able to simulate the charge dynamics because all the final state, apart from a negligible number, are not available. Since the check of the Pauli principle is done not only after the scatterings but also on the end of the free flights before the scattering, and the final states result almost always occupied, nothing happens,
any particle is able to move and the initial Fermi-Dirac distribution remains almost unchanged. This fact is explicitly underlined also in [9]. As consequence, the energy has only a perturbation around the initial mean value and the same is for the mean velocity whose perturbation is towards negative values, as shown in Fig. 8. A physical incoherence arises when the particles have to been considered near the temporal edge $\Delta t$; the free flight should end at $t^* = t + dt$ and not at $\Delta t$ and the Pauli principle should be checked at $t^*$ and not at $t = \Delta t$;

Table 3: Number of accepted and total scatterings and their ratio in the EMC with the residual time possibility simulations after 5 ps, $\varepsilon_F = 0.6$ eV, $E = 20$ kV/cm.
Figure 6: Average energy and velocity for EMC without a) and with b) the possibility of residual time $t_{res}$.
the impossibility to overcome the time edge is due to the Monte Carlo method in itself, but the FFMC does not prescribe anything for the intermediate time; it is evident that it assumes a “quantum” free flight but at the same time the $dt$ is considered in a global way and the “quantum” behaviour restricted only at its end; in this way, it seems that the time is considered at the same time both as a dynamical operator and as a parameter, subject to a boolean yes/not effect, when the Pauli principle is respected only at the end of the free flight or not, respectively. Such a situation seems to be really inconsistent from a physical point of view.

The small perturbation of the charge distribution, mean energy and velocity around the initial ones (Fig.s 7 b)-8) can be easily explained as an effect of the inclusion of the anisotropy of the phonon branches, which does not affect the EMC and DSMC results, as Fig.s 7 c) and 9 show. When the anisotropy is neglected any variation is evident. This fact should theoretically be further investigated.

To overcome the previous difficulties arising with an initial Fermi-Dirac distribution, in [9] it is proposed to use as initial condition the Maxwell-Boltzmann distribution:

$$f(0,\mathbf{k})_{MB} = \exp\left(-\frac{\varepsilon(\mathbf{k})}{k_B T^*}\right).$$

(13)

with a very high temperature $T^* = 80 \times T$ in order to reach sufficiently fast at the given field a hot Fermi-Dirac one. This choice is unphysical because $T^*$ it is much larger than the melting temperature both of silicon and graphene. For this reason in computation we must keep the phonons distributions at room temperature without any thermodynamical interaction between the electron gas and the crystal lattice. This approximation could be excessively limiting when one wants to couple the dynamics of the phonons to the charge one and to study thermal effects (see [17] [18]). Moreover, the expectation to reach the Fermi-Dirac distribution, that is an equilibrium one, is justified when any ex-
Figure 7: Distribution functions at $t = 0$ ps a) and after 5 ps for the FFMC with the Fermi-Dirac initial condition, when the phonon anisotropy is taken into account b) and not c), respectively.
Figure 8: Mean energy a) and velocity b) for the FFMC with the Fermi-Dirac initial condition when the phonon anisotropy is considered.
Figure 9: Mean energy a) and velocity b) for the FFMC with the Fermi-Dirac initial condition when the phonon anisotropy is neglected.
ternal applied electric field is considered. Therefore it can be only considered as a computational trick to get around the impossibility of considering the appropriate initial distribution of a degenerate gas. However, we perform the FFMC simulations at different values of the temperature of the initial Maxwell-Boltzmann distribution, $T^* = cT$, with $c = 1, 5, 10, 20, 40, 80$. In Fig.10 the mean energies and velocities for each case are shown, and the DSMC results are reported for comparison.

At high values of the temperature, the mean energy shows the same behaviour as in Fig.8 a); it keeps the initial value but this is very different from that obtained with the initial Fermi-Dirac (FD) distribution even when, for $T^* = 80 \times T$, it has the same shape of the Maxwell-Boltzmann (MB) one. They describe the same probability distribution but their moments are totally different. For the lower values of $c$, when the charge dynamics is in some way not frozen, the time evolution of the energy is comparable with the DSMC one, after a transient it reaches a constant value, also the variation is the same, but the starting and final values are definitively different. It is worth noting that for $c = 20$, when the zeroth order moments of the FD and MB distributions are almost equal (they are equal for $c = 16.92$) also the final value of energy-moments are almost equal; it could seem that a convergence can be exist but the Fig.10 b) shows that this result is not obtained for the mean velocity. For $c = 20$, the velocity reaches also negative values; when $c$ is increased the “quantum” treatment of the free flight works as a barrier for the charged particles that are pushed back, until for higher values of the temperature, $c = 40, 80$, nothing is allowed. Also the previous relaxation of the energy towards the DSMC value can be explained as the result of these push-backs. As expected, any equivalence with the Fermi-Dirac initial distribution is achieved and the results depend on the temperature of the initial MB distribution.

We further investigate the behaviour of the approximation of the initial Fermi Dirac distribution with a MB one when the external applied electric field is equal to zero and a convergence is expected. As shown in Fig.11 even in this case, the steady state behaviour is different for each initial MB distribution.
Figure 10: Mean energy and velocity for the FFMC with an initial Maxwell-Boltzmann distribution at different temperatures $T^* = c \times T$, $\varepsilon = 0.6 \text{ eV}$ and $E=20 \text{ kV/cm}$. 
and there is no equivalence with the FD one, represented with dot curve in Fig.11. Some kind of a convergence could be derived for $c = 16.92$ but it would be a particular case due to the equality of the number of particles and not really a convergence, that should be independent from the starting values. Besides, the values are worse when the Maxwell-Boltzmann distribution at high temperatures approximates better the Fermi Dirac one. This is a really strange and unexpected result.

For a better understanding we use as initial distribution the MB one also for the reference EMC and DSMC schemes. The DSMC simulations are performed with a constant applied electric field and with an external electric field equal to zero, respectively. In Fig.12 the mean energies and velocities do not show any convergence with respect to the values of the temperature of the MB initial distribution and this is correct because the applied electric field is not zero but the difference with the solution obtained starting from a FD distribution is higher when the MB one should better replace the FD. The results obtained with a zero electric field, Fig.13, show a convergence towards the Fermi-Dirac solution for the velocity, even if this could be only due to the small perturbation around the steady state of each case separately. Indeed, there isn’t any kind of convergence towards an equilibrium solution obtained with the FD for the mean energies. Also this time the discrepancies are greater for the higher values of $c$. The simulations based on the EMC scheme have the same behaviour of the DSMC ones as well, see Fig.14-15.

These results could seem in contradiction with the energy equipartition theorem and the markovianity of the Monte Carlo method. The latter is still valid but the standard particle based equipartition theorem no longer holds for graphene as recently stated in [20, 21] also on the basis of experimental measurements [22].

The FFMC scheme for the Monte Carlo method suffers also from some numerical instabilities; see Appendix 7 for more details. The numerical convergence of the DSMC method is analyzed in [19] when also the phonon transport in considered; the results about the good numerical convergence of the EMC
and DSMC methods both with respect the time step and the number of the simulated (super)-particles are not included at this stage for the sake of simplicity.

5 Conclusions

The Monte Carlo method has been become a standard technique for the solution of the Boltzmann equations for charge transport in semiconductors. Already from the first attempts some drawbacks have arisen. In particular the EMC method [3] is not able to determine a correct reconstruction of the charge distribution function, values greater than the maximum one are obtained and the Pauli principle is not correctly taken into account. This inconvenience is no longer negligible for the newest low dimensional materials and in all the cases the degeneracy effects are relevant. A lot of attempts were made to solve the problem by means of different approaches, all based on some approximation of the distribution function inside the scattering rate or on the scattering processes themselves. Recently, in [8], a new DSMC scheme able to properly take into account the Pauli principle has been developed; it is based on any approximation but only on an intrinsically consistent mathematical procedure. The EMC is physically consistent but it is not mathematically able to handle the limits of discretization and as consequence it produces unphysical results. The new DSMC scheme respects both the physics and the mathematics of the Boltzmann equation and clearly distinguishes the effect of the Liouville operator on the distribution function, which is treated as a whole in the free flight step, and the scattering processes that are instantaneous for the Born approximation. For both the EMC and the DSMC methods the synchronization of the particles plays a fundamental role.

In [9], an original attempt to solve the EMC problems is based no longer on the collisional operator and on the distribution functions but on the free flight steps. The Pauli principle is imposed by means of a rejection technique not only on the final states after a scattering event but also at the end of the free flight of each particle. Several mathematical and physical problems have been
Figure 11: Mean energy and velocity for the FFMC with an initial Maxwell-Boltzmann distribution at different temperatures $T^* = c \times T$, with $\varepsilon = 0.6$ eV and E=0 kV/cm.
Figure 12: Mean energy and velocity for the DSMC with an initial Maxwell-Boltzmann distribution at different temperatures $T^\ast = c \times T$, with $\varepsilon = 0.6$ eV and E=2 kV/cm.
Figure 13: Mean energy and velocity for the DSMC with an initial Maxwell-Boltzmann distribution at different temperatures $T^* = c \times T$, with $\varepsilon = 0.6$ eV and $E=0$ kV/cm.
Figure 14: Mean energy and velocity for the EMC with an initial Maxwell-Boltzmann distribution at different temperatures $T^* = c \times T$, with $\varepsilon = 0.6 \text{ eV}$ and $E = 2 \text{kV/cm}$.
Figure 15: Mean energy and velocity for the EMC with an initial Maxwell-Boltzmann distribution at different temperatures $T^* = c \times T$, with $\varepsilon = 0.6 \text{ eV}$ and $E=0 \text{ kV/cm}$. 
highlighted above.

The Fermi Dirac distribution cannot be used as the initial one and it is replaced by a Maxwell-Boltzmann distribution at high temperature. This is a computational trick that in principle can not be allowed when an electric field is applied; besides, the results strongly depend on the temperature. This aspect is fundamental for all the highly degenerate materials and above all for graphene because in this case the equipartition theorem seem to need to be reformulated.

Moreover, the free flight based Monte Carlo method reveals intrinsic physical inconsistencies, particularly with regard to time. The time is treated with a double nature of a dynamical variable when all the states before the end of the free flight are allowed and as a parameter, in a quantum perspective, when at the end of the free flight the Pauli principle is assumed to must hold.

Even if in [4] a general observation on the theoretical impossibility of the free flight to produce unphysical result on the distribution function is underlined and then the Pauli principle at the end of the free flight is considered as a purely computational solution, and the free flight based Monte Carlo is often cited, in literature there is a great amount of discussions about the approaches based on the approximation of the distribution function but any consistent analysis of the previous method, both from a mathematical point of view and about its physical implications, has been developed.

In this paper we want to remedy this lack and we highlight the strong implications and inconsistencies that the previous method shows and that are worth further investigating.

Besides, a parallel comparison with the first EMC method and the new DSMC one revealed to be of fundamental importance for a clear and as more conclusive as possible definition of the Monte Carlo method properties.

6 Acknowledgments

The author acknowledges the financial support of Progetto Giovani 2019-GNFM-InDAM.
7 Appendix: Numerical convergence of the FFMC method

The FFMC method has good convergence properties when the Fermi-Dirac distribution is assumed as initial one, as shown in Figs. 16-17, even if the convergence is less fast than the EMC and DSMC methods one. There is some instability when the Maxwell-Boltzmann distribution is used (Figs. 18-23). For $c = 80$, Figs. 22-23, the problem is not interesting because the values are almost constant. When $c = 1$, for the smallest value of $\Delta t$, a numerical instability arises when the electric field is not considered, Fig. 19; the same behaviour is present for the mean velocity when $c = 20$ and $E = 2$ kV/cm, Fig. 20 b) and $E = 0$ kV/cm, Fig. 21.

References

[1] S. Bosi and C. Jacoboni 1976 J. Phys. C: Solid State Phys. 9 315

[2] C. Jacoboni and L. Reggiani, “The Monte Carlo method for the solution of charge transport in semiconductors with applications to covalent material”, Rev. Mod. Phys., vol. 55, pp. 645-705, July 1983.

[3] P. Lugli and D. K. Ferry, “Degeneracy in the ensemble Monte Carlo method for high-field transport in semiconductors”, IEEE Transactions on Electron Devices, vol. 32, no. 11, pp. 2431-2437, Nov. 1985, doi: 10.1109/T-ED.1985.22291.

[4] P. Borowik, J. L. Thobel, Improve Monte Carlo method for the study of electron transport in degenerate semiconductors, J. Appl. Phys. 84 (1998) 3706.

[5] P. Borowik, L. Adamowciz, Improved algorithm for Monte Carlo studies of electron transport in degenerate semiconductors, Physica B 365 (2005) 235–239.
Figure 16: Mean energy and velocity for the FFMC with an initial FD at different time steps $\Delta t$, with $\varepsilon = 0.6$ eV and $E=2$ kV/cm.
Figure 17: Mean energy and velocity for the FFMC with an initial FD at different time steps $\Delta t$, with $\varepsilon = 0.6$ eV and $E=0$ kV/cm.
Figure 18: Mean energy and velocity for the FFMC with an initial MB with $c = 1$ at different time steps $\Delta t$, with $\varepsilon = 0.6$ eV and $E=2$ kV/cm.

Figure 19: Mean energy and velocity for the FFMC with an initial MB with $c = 1$ at different time steps $\Delta t$, with $\varepsilon = 0.6$ eV and $E=0$ kV/cm.

Figure 20: Mean energy and velocity for the FFMC with an initial MB with $c = 20$ at different time steps $\Delta t$, with $\varepsilon = 0.6$ eV and $E=2$ kV/cm.
Figure 21: Mean energy and velocity for the FFMC with an initial MB with $c = 20$ at different time steps $\Delta t$, with $\varepsilon = 0.6$ eV and $E=0$ kV/cm.

Figure 22: Mean energy and velocity for the FFMC with an initial MB with $c = 80$ at different time steps $\Delta t$, with $\varepsilon = 0.6$ eV and $E=2$ kV/cm.

Figure 23: Mean energy and velocity for the FFMC with an initial MB with $c = 80$ at different time steps $\Delta t$, with $\varepsilon = 0.6$ eV and $E=0$ kV/cm.
[6] M. V. Fischetti, S. E. Laux, Monte Carlo analysis of electron transport in small semiconductor devices including band-structure and space-charge effects, Phys. Rev. B 38 (1988) 9721

[7] M. Zebarjadi, C. Bulutay, K. Esfarjani, A. Shakouri, Monte Carlo simulation of electron transport in degenerate and inhomogeneous semiconductors, Appl. Phys. Letters 90 (2007) 092111.

[8] Romano, V., Majorana, A., and Coco, M., 2015, “DSMC Method Consistent With the Pauli Exclusion Principle and Comparison With Deterministic Solutions for Charge Transport in Graphene” J. Comput. Phys., 302, pp. 267–284.

[9] P. Tadyszak, F. Danneville, A. Cappy, L. Reggiani, L. Varani, and L. Rota, “Monte Carlo calculations of hot-carrier noise under degenerate conditions”, Applied Physics Letters 69, 1450 (1996); doi: 10.1063/1.117611.

[10] M. Coco, A. Majorana, V. Romano. “Cross validation of discontinuous Galerkin method and Monte Carlo simulations of charge transport in graphene on substrate”. Ricerche Mat. (2017) 66:201-220.

[11] M. Coco, A. Majorana, G. Nastasi, V. Romano. “High-field mobility in graphene on substrate with a proper inclusion of the Pauli exclusion principle”. Atti della Accademia Peloritana dei Pericolanti, Classe di Scienze Fisiche, Matematiche e Naturali, ISSN 1825-1242, Vol. 97, No. S1, A6 (2019), DOI: 10.1478/AAPP.97S1A6.

[12] P. Lichtenberger, O. Morandi, F. Schürrer, High-field transport and optical phonon scattering in graphene, Phys. Rev. B 84 (2011) 045406

[13] Castro Neto, A. H., Guinea, F., Peres, N. M. R., Novoselov, K. S., Geim, A. K. (2009). The electronic properties of graphene. Rev. Mod. Phys. 81: 109–162.

[14] Das Sarma, S., Adam, S., Hwang, E. H., Rossi, E. (2011). Electronic transport in two-dimensional graphene. Review of Modern Physics 83: 407-407.
[15] X. Li, E. A. Barry, J. M. Zavada, M. Buongiorno Nardelli, K. W. Kim, Surface polar phonon dominated electron transport in graphene. Appl. Phys. Lett., 97, 232105 (2010)

[16] K. M. Borysenko, J. T. Mullen, E. A. Barry, S. Paul, Y. G. Semenov, J. M. Zavada, M. Buongiorno Nardelli, K. W. Kim, First-principles analysis of electron-phonon interactions in graphene. Phys. Rev. B 11, 121412(R) (2010)

[17] M. Coco, V. Romano. “Simulation of electron-phonon coupling and heating dynamics in suspended monolayer graphene including all the phonon branches”. J. Heat Transfer. 2018; 140(9):092404-092404-10. doi:10.1115/1.4040082.

[18] M. Coco, G. Mascali, V. Romano. “Monte Carlo analysis of thermal effects in monolayer graphene”. Journal of Computational and Theoretical Transport, Vol. 45 (7): 540-543 (2016).

[19] M. Coco, V. Romano. “Assessment of the constant phonon relaxation time approximation in electron-phonon coupling in graphene”. Journal of Computational and Theoretical Transport. 7 (1-3), 246–266, 2018. doi: 10.1080/23324309.2018.1558253.

[20] Hosang Yoon and Donhee Ham, Massive thermal fluctuation of massless graphene electrons. [arXiv:1405.2356v2].

[21] Yoon, Hosang. 2014. Two-Dimensional Plasmonics in Massive and Massless Electron Gases. Doctoral dissertation, Harvard University. [http://nrs.harvard.edu/urn-3:HUL.InstRepos:13070026]

[22] H. Yoon, C. Forsythe, L. Wang, N. Tombros, K. Watanabe, T. Taniguchi, J. Hone, P. Kim, and D. Ham, Nature Nanotechnology advance online publication (2014), 10.1038/nnano.2014.112.
[23] Ferry D.K., Goodnick S.M. (2001) Ensemble Monte Carlo Simulations of Ultrafast Phenomena in Semiconductors. In: Tsen KT. (eds) Ultrafast Phenomena in Semiconductors. Springer, New York, NY.

[24] A. Islam, K. Kalna, Monte Carlo simulations of mobility in doped GaAs using self-consistent Fermi–Dirac statistics, 2011 Semicond. Sci. Technol. 26 055007.