Particle dynamics in graphene - Collimated beam limit

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Abstract

We investigate the particle dynamics in a two-dimensional structure containing two different populations of particles. We consider the semiclassical high temperature limit of the particle gas. The particle motion is described at the hydrodynamic level. We show the existence of a regime, denoted as collimated beam limit, where the problem of the closure of the hydrodynamic moments hierarchy simplifies considerably. Some numerical experiments are presented where our model is applied to the numerical simulation of a nanometric device based on a graphene sheet.

1 Introduction

Graphene denotes a monoatomic layer of graphite. It is a 2-dimensional material with extraordinary mechanical and electrical properties. In particular, the interesting electronic properties of graphene derive from the conical shape of energy bands in the proximity of the so-called Dirac points. Close to such points, the electron wave function is described by the Dirac-like relativistic Hamiltonian [3]

\[ H(x, p) = cp \cdot \sigma + V(x). \] (1)

Here, \( x = (x_1, x_2, 0) \) and \( p = (p_1, p_2, 0) \) are the coordinates of the electron position and momentum, \( c \approx 10^6 \text{ m/s} \) is the Fermi velocity, \( V(x) \) is the electrostatic potential that includes external and self-consistent fields and, as usual, \( \sigma = (\sigma_1, \sigma_2, \sigma_3) \) is the vector of Pauli matrices. Note that, according to (1), electrons in graphene behave like photons or neutrinos, with an “effective light speed” \( c \), which is about 1/300 of the speed of light in vacuum, and subject to electric forces. The spin-like degree of freedom associated to the Hamiltonian (1) is called “pseudospin” and arises from the decomposition of the graphene honeycomb lattice into two non-equivalent triangular lattices [3] (note that the continuous degrees of freedom (\( x \) and \( p \)) are 2-dimensional, while the pseudospin vector is 3-dimensional). Graphene, therefore, can be considered as an ideal laboratory where quantum-relativistic effects can be studied at non-relativistic energies [6].

The electronic energy bands are the eigenvalues of \( H \) evaluated at \( V = 0 \) and are given by

\[ E_{\pm}(p) = \pm c|p|, \] (2)

showing the above-mentioned conical shape. The semiclassical velocities associated to the energy bands (2) are

\[ \nabla_p E_{\pm}(p) = \pm c \frac{p}{|p|}, \] (3)
which implies that, from a semiclassical viewpoint, electrons move at constant speed $c$.

In this paper we deal with a hydrodynamic model for electron transport in graphene derived in Ref. [1], focusing in particular on the equations for the “collimated beam” limit.

In Section 2 we summarize the derivation, obtained in Ref. [1], of a hydrodynamic system describing a population of electrons or holes in graphene. We derive the mathematical formulation of the problem in the framework of the kinetic description of the quantum particle dynamics, represented by the Wigner equations endowed with a BGK relaxation term. The maximum entropy principle [13, 10, 11] allows to close the hierarchy of moment equations. In Section 3, the general system presented in Sec. 2 is specialized to the case of high temperature (which is equivalent to using Maxwell-Boltzmann statistics) and, more in particular, to the so-called “collimated-beam limit”. Such limit corresponds to a distribution of carriers having (locally) all the same direction. It is shown that such a system has the properties of a geometrical-optics system, with the electric potential playing the role of the refractive index. Finally, in Section 4, some numerical tests on the collimated-beam equations are discussed. These experiments highlight some interesting properties of such system, such as the formation of shock waves, the influence of the component of the electric field orthogonal to the beam and the deflection of trajectories by a potential barrier.

2 Hydrodynamic equations

We give here the derivation of the hydrodynamic model for graphene. Let us consider the transport equations for a statistical population of electrons in graphene. These are given by the Wigner equations associated to the Hamiltonian (1) that we write here in semiclassical form

\[\begin{align*}
\partial_t w_0 + c \nabla_x \cdot w + F \cdot \nabla_p w_0 &= \frac{1}{\tau} (w_{0}^{\text{eq}} - w_0), \\
\partial_t w + c \nabla_x w_0 + F \cdot \nabla_p w - \frac{2c}{\hbar} p \times w &= \frac{1}{\tau} (w_{0}^{\text{eq}} - w),
\end{align*}\]

\( (4) \)

developed by the external force. The right side of (4) takes into account the interactions of the electrons with the environment (the detailed description of all the relevant relaxation processes can be found in Ref. [7]). The collisional interactions are modeled by a BGK term and describes the relaxation of the electron population to a local-equilibrium state $w_{0}^{\text{eq}}$ in a characteristic time $\tau$. Denoting the direction of the momentum by $\nu$,

\[\nu(p) = \frac{p}{|p|} = (\nu_1(p), \nu_2(p), 0),\]

\( (5) \)

it is known from general theory [2] that

\[w_{\pm} = \frac{1}{2} (w_0 \pm \nu \cdot w),\]

\( (6) \)

can be semiclassically interpreted as the phase-space densities of electrons with, respectively, positive and negative energies, i.e. belonging to the upper and the lower cones of (2). The equations for $w_+$ and $w_-$ can be readily deduced from (4) and read as follows:

\[\begin{align*}
(\partial_t \pm c \nu \cdot \nabla_x + F \cdot \nabla_p) w_\pm + c \nabla_x \cdot w_\pm \pm \nu \cdot (F \cdot \nabla_p) w_\pm &= \frac{1}{\tau} (w_{0}^{\text{eq}} - w),
\end{align*}\]

\( (7) \)
where $w_\perp$ denotes the projection of $w$ orthogonal to $\nu$. Due to the unboundedness from below of the Hamiltonian (1), the moments of the equilibrium distribution of electrons in the lower cone, $w_\pm^\perp$ are divergent. Then, lower-cone electrons require a description in terms of electron vacancies, i.e. holes, which can be introduced by denoting

$$f_+(p) = w_+(p), \quad f_-(p) = 1 - w_-(p).$$

The equations for $f_+$ and $f_-$ are

$$(\partial_t + c\nu \cdot \nabla_x \pm F \cdot \nabla p) f_\pm + c \nabla_x \cdot w_\perp \pm \nu \cdot (F \cdot \nabla p) w_\perp = \frac{1}{\tau} (f_\pm^\text{eq} - f_\pm),$$

where now the local-equilibrium distributions of electrons in the upper cone, $f_+^\text{eq}(p) = w_+^\text{eq}(p)$, and holes in the lower cone, $f_-^\text{eq}(p) = 1 - w_-^\text{eq}(-p)$, have both finite moments (if Fermi-Dirac statistics is assumed). According to the maximum entropy principle, in Ref. [1] it is proven that in the hydrodynamic limit $\tau \to 0$ we have

$$f_\pm \to f_\pm^\text{eq}, \quad \text{and} \quad w_\perp \to 0$$

and then we obtain

$$(\partial_t + c\nu \cdot \nabla_x \pm F \cdot \nabla p) f_\pm^\text{eq} = 0.$$

Differing from the full quantum regime [8], as it can be seen from Eq. (10), the electrons and holes are decoupled in the hydrodynamic limit, then, in order to avoid cumbersome notations, we shall suppress henceforth the $\pm$ labels everywhere and the equations for electrons and holes will be identified only by the charge sign (i.e. by the sign of the force terms). Moreover, since the pseudospin ceases to play any role, the vectors will be all 2-dimensional from now on.

The hydrodynamic description we are going to introduce is based on the following moments: electron/hole density

$$n = \langle f_\text{eq} \rangle,$$

electron/hole density

$$u = \left( \frac{\nu f_\text{eq}}{n} \right)$$

electron/hole direction field

(so that $cu$ is the average velocity field), where we put

$$\langle g \rangle = \frac{1}{(2\pi \hbar)^2} \int_{\mathbb{R}^2} g(p) \, dp$$

for any scalar or vector-valued function $g$ of $p \in \mathbb{R}^2$. As a straightforward consequence of Jensen’s inequality we have that

$$|u| \leq 1.$$ (13)

According to above-mentioned maximum entropy principle (MEP), the local-equilibrium state $f_\text{eq}$ is the most probable microscopic state with the observed macroscopic moments $n$ and $u$. “Most probable” means that it maximizes a suitable entropy functional which, assuming that the system is in thermal equilibrium with a phonon bath at temperature $T$, is (minus) the free-energy [10]

$$\mathcal{E}(W) = \int_{\mathbb{R}^4} [k_B T s(f) - E f] \, dp \, dx,$$ (14)
where $E = c|p|$, $k_B$ is the Boltzmann constant and $s(f) = -f \log f - (1 - f) \log(1 - f)$ is the Fermi-Dirac entropy function. It can be proven that such a maximizer has the form

$$f_{eq} = \frac{1}{e^{\frac{|p| - \nu \cdot B - A}{k_B T}} + 1},$$

(15)

where $A$ and $B = (B_1, B_2, 0)$ are Lagrange multipliers.

By taking the moments $\langle \cdot \rangle$ and $\langle \nu \cdot \rangle$ of Eq. (10), and using (11), we obtain the moment equations

$$\begin{aligned}
&\partial_t n + c \partial_i (nu_i) = 0, \\
&\partial_t (nu_i) + c \partial_j P_{ij} = \pm F_j Q_{ij},
\end{aligned}$$

(16)

where $\partial_i = \partial/\partial x_i$ and

$$P_{ij} = \langle \nu_i \nu_j f_{eq} \rangle, \quad Q_{ij} = \langle \frac{\partial \nu_i}{\partial p_j} f_{eq} \rangle = \langle \frac{1}{|p|} \nu^*_i \nu^*_j f_{eq} \rangle$$

(17)

(with $\nu_\perp = (-\nu_2, \nu_1)$).

Note that the implicit closure of this system is provided by the fact that the Lagrange multipliers $A$ and $B$ in $f_{eq}$ depend on the moments $n$ and $u$ through the constraints (11). Then, Eqs. (11), (15), (16) and (17) is a “closed” hydrodynamic model for electrons/holes in graphene. Such system can be proven to be hyperbolic [1] and then it is, at least, locally well-posed.

The expression of the Lagrange multipliers $A$ and $B$ as functions of $n$ and $u$ cannot be explicitly obtained, in general, but system (11) can be further simplified. In fact, it is not difficult to prove that the direction of $B$ coincides with the direction of $u$. We introduce the functions

$$I^s_N(A,B) = \frac{1}{\pi} \int_0^\pi \cos(N\theta) \phi_s(A + B \cos \theta) d\theta,$$

(18)

where $A \in \mathbb{R}$, $B \geq 0$, $s > 0$, $N \in \mathbb{Z}$, and

$$\phi_s(x) = \frac{1}{\Gamma(s)} \int_0^\infty \frac{t^{s-1}}{e^t - x + 1} dt.$$

(19)

$\phi_s$ is the so-called Fermi integral of order $s$. Equation (11) can be reduced to a system of just two scalar equations, relating $n$ and $|u|$ to $A$ and $B = |B|:

$$I^2_0(A,B) = \frac{2\pi \hbar^2 c^2 n}{(k_B T)^2}, \quad \frac{I^2_1(A,B)}{I^2_0(A,B)} = |u|$$

(20)

Moreover, the moments $P_{ij}$ and $Q_{ij}$ can be expressed in terms of the scalar Lagrange multipliers $A$ and $B$ as follows:

$$P_{ij} = \frac{n}{|u|^2} (P_{ij} + P_{\perp} u^*_i u^*_j),$$

$$Q_{ij} = \frac{c}{k_B T} \frac{n}{|u|^2} (Q_{ij} + Q_{\perp} u^*_i u^*_j),$$

(21)
where \( u^\perp = (-u_2, u_1) \) and the scalar functions \( P(A, B), P_\perp(A, B), Q(A, B), Q_\perp(A, B) \) are given by

\[
P = \frac{I_0^2 + I_2^2}{2I_0^2}, \quad P_\perp = \frac{I_0^2 - I_2^2}{2I_0^2} = 1 - P, \\
Q = \frac{I_0^1 - I_2^1}{2I_0^2}, \quad Q_\perp = \frac{I_0^1 + I_2^1}{2I_0^2}
\]

(and \( I_N = I_N^\perp(A, B) \)). Then, the problem of giving the hydrodynamic model (11), (15), (16), (17) an explicit form is reduced to the problem of computing \( P, P_\perp, Q, Q_\perp \) as functions of \( n \) and \( |u| \), through system (20). Even though this program cannot be carried out in general, nevertheless special regimes (of physical relevance) exist where the explicit expressions can be obtained [1]. In the next section one of these cases will be examined, namely the limit of high temperatures.

3 Maxwell-Boltzmann limit

Let us consider the form of the hydrodynamic model (11), (15), (16), (17) as \( T \to \infty \). From Eq. (20) we see that this corresponds to studying the asymptotic \( I_0^2 \to 0 \). Since it is known that \( \phi_s(x) \to 0 \) if and only if \( x \to -\infty \), it is clear that \( I_N^2(A, B) \to 0 \) if and only if \( A \to -\infty \) and \( B < -A \). Moreover, we can use the asymptotic approximation [12]

\[
\phi_s(x) \sim e^x, \quad \text{as} \quad x \to -\infty.
\]

From (18) we see, therefore, that

\[
I_N^s(A, B) \sim e^A I_N(B), \quad \text{as} \quad A \to -\infty \text{ and } B < -A,
\]

where \( I_N \) denotes the modified Bessel function of the first kind of order \( N \). This asymptotic expression greatly simplifies the mathematical structure of the problem, first of all because of its factorized structure and, secondly, because the dependence on \( s \) has disappeared. It can be easily seen that using Eq. (23) corresponds to approximating \( f_{\text{eq}} \) with the Maxwell-Boltzmann distribution

\[
f_{\text{eq}} \sim e^{-\frac{1}{\beta} E + \nu \cdot B + A}.
\]

By using (23), the constraint equations (20) become

\[
e^A I_0(B) = \frac{2\pi \hbar^2 c^2 n}{(k_B T)^2}, \quad \frac{I_1(B)}{I_0(B)} = |u|.
\]

Note, in particular, that \( B \) only depends on \( |u| \). Moreover, the coefficients \( P, P_\perp, Q \) and \( Q_\perp \) take the simple form

\[
P = 1 - P = Q_\perp = 1 - Q = \frac{I_0(B) + I_2(B)}{2I_0(B)}
\]

(in particular, they only depend on \( |u| \)). Then, by introducing the function \( X(|u|) \) defined by

\[
X(|u|) = \frac{I_0(B) + I_2(B)}{2I_0(B)}, \quad B = \left(\frac{I_1}{I_0}\right)^{-1}(|u|)
\]
(where we recall that $0 \leq |u| < 1$), we obtain the following explicit form of Eq. (21):

$$
P_{ij} = \frac{n}{|u|^2} \left[ X(|u|)u_i u_j + (1 - X(|u|)) u_i^\perp u_j^\perp \right],
$$

$$
Q_{ij} = \frac{c}{k_B T} \frac{n}{|u|^2} \left[ (1 - X(|u|)) u_i u_j + X(|u|) u_i^\perp u_j^\perp \right].
$$

(28)

The function $X(|u|)$ increases monotonically from $1/2$ to 1 as $|u|$ increases from 0 to 1. When $|u| \to 0$ the velocities are equally spread in all directions and we obtain a diffusive limit [1]. On the opposite side, when $|u| \to 1$, the velocities are concentrated along a $(\langle x, t \rangle$-dependent) direction in the $p$-space (the direction determined by $u$). For this reason, we denote this regime as the “collimated beam limit”. The hydrodynamic equations corresponding to such limit will be now obtained and some numerical experiments will be presented in next section.

Since $X(|u|) \to 1$ as $|u| \to 1$, from Eq. (28) we easily obtain

$$
P_{ij} \to n u_i u_j, \quad Q_{ij} \to \frac{c}{k_B T} n u_i^\perp u_j^\perp.
$$

Then, the second of equations (16) reduces to

$$
\partial_t (n u_i) + c \partial_j (n u_i u_j) = \pm \frac{c}{k_B T} n u_i^\perp F_j u_j^\perp,
$$

which, by using the continuity equation $\partial_t n + c \partial_j (n u_i)$, can be rewritten as

$$
\partial_t u_i + c u_j \partial_j u_i = \pm \frac{c}{k_B T} u_i^\perp F_j u_j^\perp.
$$

(29)

We see, therefore, that the equation for $u$ decouples from the continuity equation. A simple computation shows that Eq. (29) is compatible with the assumption of collimation. In fact, multiplying by $2u_i$ both sides of (29) and summing up over $i$ yields the equation

$$
\partial_t |u|^2 + c u \cdot \nabla |u|^2 = 0,
$$

from which it can be seen that, for any regular solution $u(x, t)$ of Eq. (29) such that $|u(x, 0)| = 1$ at the initial time $t = 0$, we have that $|u(x, t)| = 1$ for all times $t > 0$ at which the solution exists.

Let us now consider the stationary version of Eq. (29), that we rewrite as follows:

$$
(u \cdot \nabla) u \pm (u^\perp \cdot \frac{1}{k_B T} \nabla V) u^\perp = 0.
$$

(30)

Since we are assuming $|u| = 1$, then we can write $u = (\sin \varphi, \cos \varphi)$. Substituting this expression in Eq. (30), we obtain the conservation law

$$
\text{div} \left( e^{\pm \frac{1}{k_B T} V} u^\perp \right) = 0.
$$

(31)

Equation (31) reveals that the collimation regime has the properties of a geometrical-optics system, with $e^{\pm \frac{1}{k_B T} V}$ playing the role of the refractive index (we recall that $+$ refers to electrons and $-$ to holes). It is interesting to notice that, within our semiclassical model, we always find a positive refractive index but a negative refractive index may arise from a fully quantum description [4].
Figure 1: Free fly evolution of the velocity field. The panels depict the solution at different times. Panel a: initial condition. Panel b: $t = 0.2$. Panel c: $t = 0.4$. In the left (right) side is depicted the $x$ ($y$) component of the speed. Up-left panel: vectorial representation of the velocity field at different times.

4 Numerical results

We consider the following system

$$\partial_t u_i + cu_j \partial_j u_i = \frac{c}{k_B T} u_i^\perp F_j^\perp u_j^\perp ; i, j = x, y .$$

(32)

We investigate the particle dynamics inside a graphene sheet by presenting some numerical tests preformed on Eq. (32). We focus on a simple prototype of nanometric device. It is constituted by connecting a suspended graphene sheet to two ohmic contacts which are denoted as source and drain [9]. By applying an external electric field, it is possible to induce a current in the graphene sheet. We indicate the direction of the particle flow by the axis $x$ (parallel direction). The distance between source and drain spans typically from the nanometric to the micrometric size. In the ideal case, it is assumed that the graphene sheet is very large along the direction orthogonal to current flow. The effects of the edges are thus neglected. In this case, the external force field is directed along the $x$ direction and the particle density and current are independent from the orthogonal direction $y$. We obtain the
simplified system

\begin{align}
\partial_t u_x + u_x \partial_x u_x &= \gamma u_y^2 F_x \\
\partial_t u_y + u_x \partial_x u_y &= -\gamma u_x u_y F_x
\end{align}

where we used normalized units. Here, \( t_0 \) (\( l_0 \)) is the characteristic of time (length) of the system. We fix \( l_0/t_0 = c \). The dimensionless parameter \( \gamma \) is

\[ \gamma = \frac{t_0 c E_0}{k_B T} \]

where \( E_0 \) is the typical value of the electric field inside the material. In order to illustrate the results of our calculations, we consider at first the simple case of the free particle motion and we set \( F_x = 0 \). As an initial condition we consider a particle beam that travels from the left (source) to the right (drain) and whose \( x \)–velocity follows a a gaussian dispersion low in the space. Since \( |u| = 1 \), we set \( u_y(t = 0) = \sqrt{1 - u_x^2(t = 0)} \). This is illustrated in Fig. 1
Figure 3: Deviation of the particle trajectory. Lower panel: angle between the initial and the final direction of the speed for different incident angles. Upper panel: the initial (blue arrow) and the final direction of the speed (red arrow). We set $E_x = 1$.

where in the panel $a$ we depict the initial conditions of the velocities $u_x$ (left plot) and $u_y$ (right plot). The numerical approximation of the solution of Eqs. (33)-(34) is depicted in the panels $c - d$. In our simulations we set $\gamma = 1$. We display the solution for $t = 0.2$ (panel $b$) and $t = 0.4$ (panel $c$). We see that the particles travel toward the drain contact until for $t = 0.4$ a shock is formed. The formation of shock waves is a well known property of this kind of hyperbolic systems [5]. In order to ease the lecture of the numerical results, in the top-left panel of Fig. 1 we depict the two-dimensional components of the velocity field. The curve $A - A'$ indicates the trajectory of a test particle. We add now an external electric field. The profile of the electric field $F_x$ is depicted in Fig. 2 in the up-left panel (lower plot). The electric field changes the direction of the speed and causes the reflection of the particles. In the panels $a - c$ we depict the evolution of the velocity in the time interval $[0, 0.5]$. The electric force generates a negative component of the velocity along the $x$ direction. In this case, the origin of the shock wave is evident. There are two fluxes of particles that travel in opposite directions and their trajectories intersect around $x = 0$. This is illustrated in the up-left panel, where we indicates two intersecting trajectories ($A - C$ and $B - C$).

As a final example, we evaluate the deviation of the particle motion induced by the electric field. A well known property of particle dynamics in graphene is that electrons and holes pass through any potential barrier that is orthogonal to their trajectory. Electric fields which are parallel to the direction of the particle speed are unable to deflect the trajectory of the particle and the motion proceed along a straight line. This can be easily seen from the equation of motion (33)-(34). When $u_y = 0$, the right side of both equations vanishes. We illustrate this property by considering the particle motion in the presence of a constant electric field. We denote by $\alpha$ the angle formed by the particle speed and the $x$ axes. For $t = 0$ we assume that the velocity field is uniform. We solve the equation of motion and we plot the value of $\alpha$ at the final time $t_f = 0.5$. The result is depicted in Fig. 3. We plot the quantity $\alpha(t_f) - \alpha(0)$ for different values of the initial incidence direction. As expected, the direction of the motion
does not change when $\alpha = 0$. The maximum deflection is obtained for $\alpha = \pi/4$. In the upper plot we depict the initial (blue arrow) and the final direction of the speed (red arrow).

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