Wigner model for Klein tunneling in graphene

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Communicated by Roberto Natalini

Abstract
Quantum corrections to the electron-hole motion in graphene are investigated by applying the multiband Wigner approach. A diagonalization procedure regarding the pseudo-spin degree of freedom is proposed. The resulting formulation of the equation of motion reveals to be particularly close to the classical description of the particle motion. This formal analogy offers a framework in which quantum phenomena can be described with a classical language and the question of the quantum-classical correspondence can be directly investigated. Some numerical results are presented showing the ability of our quasi-diagonal Wigner model to reproduce Klein tunneling in graphene under the application of an external electric field.

Keywords: Quantum transport, Wigner formalism, Klein tunneling, graphene.

AMS Subject Classification: 81S30, 81Q15, 81S22

1. Introduction.
Graphene denotes a single layer of $sp^2$-bonded carbon atoms densely packed into a benzene-ring structure. This ideal planar structure has been used to describe properties of many carbon-based materials including graphite (that can be viewed as a large number of superposed graphene sheets). Graphene displays unusual electronic properties arising from a linear electronic band dispersion near the Brillouin zone corners (Dirac points). In a quite wide range of energy around the Dirac points, electrons and holes propagate as massless Fermions. They move through the layer with a velocity $v_F = 10^6$ m s$^{-1}$, which is 300 times smaller than the speed of light. The dispersion relation in graphene, mimics the physics of quantum electrodynamics but at the much smaller energy scale of the solid state physics. A novel set of phenomena have been recently discovered in such a material, that opens the possibility to study the implication of the
relativistic-like electron behaviour in the solid state. Some of the anomalous quantum transport properties displayed by massless particles in graphene are for example the integer quantum Hall effect and the Aharonov-Bohm effect \[1,2\]. Experimental studies revealed that quasi-ballistic transport in a graphene sheet is weakly affected by external sources of disorder (defects or impurities). For this reason, the charge mobility in graphene layers attains large values that cannot be reached in conventional semiconductors (mobility of the order of \(10^5\) cm\(^2\)V\(^{-1}\)s\(^{-1}\) have been recently measured \[3\]). In fact, Dirac fermions are quite immune to the localization effects and it has been observed experimentally that electrons can propagate without scattering over distances of the order of micrometers \[4\]. Furthermore, in high-density low-temperature regimes, the mobility is roughly density- and temperature-independent. Graphene is a semiconductor, whose band gap is exactly zero and the velocity of the charge carriers is independent of the momentum (and does not decrease at the top of the valence band as in the usual semiconductor materials). For these reasons, graphene is expected to be in a low-conductivity state when the Fermi energy approaches the Dirac point where the density of states vanishes. A gate voltage can, however, modulate the density of states in graphene and switch between the low-conductivity state at the Dirac point and the high-conductivity states elsewhere. Because of its high electronic mobility and the capability of being tuned from \(p\)-type to \(n\)-type doping by the application of a gate voltage, graphene is an interesting candidate towards possible applications in carbon-based electronics devices. In particular, some applications are already devised by various groups, for example in designing devices \[5,6\] or spin injection devices \[7\].

Experimental studies on nearly perfect graphene crystals, revealed the presence of some mechanisms limiting the electron mean free path to less than few microns. As a result, various hypotheses has been established to understand the possible presence of some intrinsic mobility-limiting mechanisms \[8\]. Although evidence has mounted that interactions with the underlying substrate are largely responsible (possible sources of scattering include adsorbents and defects in the graphene lattice, ionized impurities in the silicon oxide substrate, surface charge traps, interfacial phonons, substrate ripples \[9\]), the exact nature of the scattering that limits the mobility of graphene devices remains unclear. Consequently, progress in theoretically studying graphene could share light in this controversial field. In particular, devices where the effect of the contact between the semiconductor substrate and the graphene is minimized, as for example in high quality suspended graphene, appear as a promising configuration where a theoretical study of the dynamics of particles, which include scattering, can be addressed.
Moreover, when the Fermi level approaches the Dirac point, the density of states vanishes and it is expected that also the conductivity becomes strictly zero. On the contrary, the theoretical prediction of Fradkin, given in Ref. [10], concerning the presence of a residual minimal charge conductivity, was confirmed by experiments. The main reason of this phenomenon concerns the difficulty of localizing Dirac-like particles in a single band. The possibility to perform easily band-to-band transitions, provided by the gapless Dirac-like form of the Hamiltonian, reveals that the particles can travel over long distances (or penetrate a potential barrier) without creating a reflected component by converting itself in an electron-hole excitation. Because of the strong similarity with relativistic quantum mechanics, the tunneling of an electron through an $n-p$ graphene junction, where conduction-like states are converted into hole-like states (and vice versa), is denoted as Klein tunneling. Several recent experiments have investigated this unusual coupling of electron-like and hole-like dynamics [11]. Klein tunneling gives rise to some unusual behaviour of the charge transport when the Fermi level approaches the Dirac point, where the valence and conduction bands meet. Anyway, the apparent suppression of the particle localization in graphene is a phenomenon under study and its microscopical explanation is still unclear.

In solid state physics, we are typically interested in macroscopic phenomena which are slowly varying in time and smooth in space apart from variations on the atomic scales. The language used to describe electron transport is derived from the semi-classical picture of the dynamics where the electrons respond to external fields like point particles. The development of efficient quantum computational methods is thus a crucial aspect in the study of new devices where quantum-mechanical effects play a dominant role. Different approaches based on the density matrix, non-equilibrium Green’s functions, and the Wigner function have been proposed to achieve a full quantum description of the electron transport [12]. Among them, the Wigner-function formalism is the one that bears the closest similarities to the classical Boltzmann equation, so that this formalism can be considered as a natural choice to derive quantum corrections to the classical phase-space motion. Furthermore, a phase-space approach may appear more intuitive compared with the more abstract density matrix and Green’s function formalism. The phase-space formulation of quantum mechanics offers a framework in which quantum phenomena can be described with a classical language and the question of the quantum-classical correspondence can be directly investigated. For these reasons, an approach where both the kinetic characteristic of the particles and the pseudospin degree of freedom are described in a full-quantum framework, seems to be a promising approach to...
share light on this unusual property of graphene. Anyway, the close similarity between the classical mechanics and a quantum kinetic framework which characterizes the Wigner single-band formalism, is generally lost when we address the many-band dynamics. In fact, a straightforward extension of the standard definition of the Wigner function, leads to very complicated multi-band systems, where a one-to-one relationship between band and distribution function cannot be found. In general, it is not possible to define a quasi-distribution function associated to a single kind of particle (hole or electron) and whose marginal distribution (for example the integral with respect the momentum) represents some expectation value of such a particle.

In this contribution, we study the effect of Klein tunneling, and we present a Wigner-like multiband formalism. In sec. 2 the derivation of the quasi-diagonal equations of motion is presented and our approach is compared with some preexisting methods. In sec. 2.3 the numerical difficulties related to a direct solution of the transport equations are discussed and in sec. 2.5 some asymptotic approaches are proposed. Finally, in sec. 2.5.1 we apply our formalism to reproduce Klein tunneling in graphene.

2. Model.

Graphene is the ideal bidimensional allotropic form of carbon, where the atoms are periodically arranged in a honeycomb-lattice. Such an atomic structure is characterized by two types of bonds and exhibits the so-called planar sp² hybridization. The σ bonds are strong covalent bonds responsible for most of the binding energy and for the elastic properties of the graphene sheet. However, since the upper (lower) bound of the σ (σ*) band is quite far away the Fermi energy (more than 4 eV and 8 eV at the Γ point for the σ and the σ* orbital, respectively), bonding and anti-bonding σ bands can be safely neglected when addressing the electronic transport properties of graphene. The half-filled π bands are responsible for the charge transport properties. The first who studied the graphene band structure was P. R. Wallace in 1946 by using a tight binding approach [13]. Subsequently, more refined models were derived, providing a reliable theoretical basis for the description of the electronic properties in this material (an exhaustive bibliography concerning this models can be found in [14]). In the present work we consider the following graphene Hamiltonian [11,15]:

\[ H = H_0 + \sigma_0 U(\mathbf{r}) , \]
\[ H_0 = -i v_F \hbar \mathbf{\sigma} \cdot \nabla_{\mathbf{r}} = v_F \hbar \begin{pmatrix} 0 & -i \frac{\partial}{\partial x} - \frac{\partial}{\partial y} \\ -i \frac{\partial}{\partial x} + \frac{\partial}{\partial y} & 0 \end{pmatrix}, \]
which describes the motion of an electron-hole pair in a graphene sheet lying
on the \((x-y)\) plane, in the presence of an external potential \(U(r)\). Here \(v_F\) is
the Fermi velocity, \(\sigma = (\sigma_x, \sigma_y, \sigma_z)\) is the Pauli matrices-vector, where \(\sigma_x =
\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},\) and \(\sigma_0\) denotes the identity \(2 \times 2\)
matrix. The valence and conduction bands are usually denoted as pseudo-
spin components of the particle and the form of the coupling between them
can be interpreted as an effective momentum-dependent magnetic field \(\mathbf{h} \propto \sigma \cdot \nabla r\).

2.1. Quasi-diagonal Wigner evolution equation.

In this section we derive the equation of motion of the particles in
the quantum kinetic formalism by defining a suitable quasi-diagonal multi-
component Wigner function. The Wigner function for a multiband system
is defined as

\[
\mathbf{f}_{ij}(\mathbf{r}, \mathbf{p}) = \frac{1}{(2\pi \hbar)^2} \int \psi_i(\mathbf{r} + \frac{\eta}{2}) \psi_j(\mathbf{r} - \frac{\eta}{2}) e^{-i \frac{\mathbf{p} \cdot \eta}{\hbar}} d\eta,
\]

where \(\Psi = \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}\) is the two component Schrödinger wave function satisfying
\(i\hbar \frac{d\Psi}{dt} = \mathcal{H}\Psi\). Equation (3) is a straightforward extension of the single band
Wigner function, where the Wigner transformation is applied component-
wise to the density matrix. Up to the first order in \(\hbar\), the equation of motion
for the multi-component Wigner function writes

\[
\begin{align*}
\frac{\partial \mathbf{f}^S(\mathbf{r}, \mathbf{p})}{\partial t} &= -\frac{v_F}{2} \nabla_r f_0 + (\nabla_r U \cdot \nabla_p) \mathbf{f}^S + \frac{v_F}{\hbar} \mathbf{f}^S \wedge \mathbf{p} \\
\frac{\partial f_0(\mathbf{r}, \mathbf{p})}{\partial t} &= \nabla_r U \cdot \nabla_p f_0 - \frac{v_F}{2} \text{div} \mathbf{f}^S
\end{align*}
\]

where we defined the vector \(\mathbf{f}^S = (2\Re \{f_{21}\}, 2\Im \{f_{21}\}, f_{11} - f_{22})\), \(f_0 = f_{11} + f_{22}\) and \(\Im (\Re)\) denotes the imaginary (real) part. The formulation of the
multi-band Wigner approach given in Eqs. (4)-(5) is characterized by the
presence of high oscillating regimes making its numerical treatment a very
difficult task. This behaviour is caused by a strong entanglement between
the transition band phenomena (whose frequency is proportional to the en-
ergy difference between states localized in the upper and the lower Dirac
cones) and the intraband motion of the electrons (that, with respect to the
tunneling processes, can be considered as a slow dynamical process). Fur-
thermore, in this formulation the analogy with the semi-classical evolution
of the system (characterized by two uncoupled Liouville equations, one for
the particle distribution function in the upper cone, and one for the hole dis-
tribution function in the lower cone) is completely lost. Here, a description
of the dynamics where we can associate a certain quasi-distribution function to the particle and a different quasi-distribution function to the holes, does not applies. One of the most remarkable advantage of the single-band Wigner formulation of the quantum mechanics (and was the main reason for which this formulation has been introduced) is that in this framework the classical limit $\hbar \to 0$ is easily evaluated. As showed by the Eqs. (4)-(5), this is no longer true in the many-band case, where the limit $\hbar \to 0$ is completely non-trivial. This is due to the presence of the last term of Eq. (4). When $\hbar$ goes to zero, the various components of $f$ become more and more coupled and the system becomes ill defined. This simple consideration suggests to use instead to $(f^S, f^0)$, some new unknowns behaving regularly in the limit $\hbar \to 0$. This can be obtained by a partial diagonalization of the equation of motion. In the following we will introduce the quantum corrections in the particle-hole system in a more tractable formulation.

2.2. Derivation of the W-MEF system.

We derive the equation of motion of particles in graphene by using an approach based on the framework of operator mechanics. We write Eqs. (4)-(5) in the compact form

$$
\hbar \frac{\partial f}{\partial t} = \left( A_0 + \hbar \mathbf{B} \cdot \mathbf{\nabla}_r + \hbar \mathbf{E} \cdot \mathbf{\nabla}_p \right) f,
$$

where $f = (f_{11} + f_{22}; f_{11} - f_{22}; 2\Im \{f_{21}\} ; 2\Re \{f_{21}\})^t$. In order to avoid confusion, we used an arrow to denote two-dimensional vectors, e.g., $\mathbf{B} = (B_x, B_y)$, and

$$
B_x = -\frac{v_F}{2} \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} ;
B_y = -\frac{v_F}{2} \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}
$$

$$
A_0 = v_F \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & -p_x p_y \\ 0 & p_x & 0 & 0 \\ 0 & -p_y & 0 & 0 \end{pmatrix}.
$$

By considering $\hbar$ as an asymptotic parameter, we search for a new set of pseudo-distribution functions, for which the zeroth-order dynamics is diagonal. We define the operator $\Theta$ acting on $f$

$$
\Theta f = \left[ \Theta^0 + \hbar \mathbf{\nabla}_r \cdot \mathbf{\nabla}_r \right] f,
$$
where the $\Theta_0^\rightarrow, \Theta_r^\rightarrow$ appearing in the previous formula, are $4 \times 4$ matrices and depend on the $x$ and $p$ variables. We choose $\Theta$ such as

$$\Theta^{-1}\left(A_0 + h \vec{B} \cdot \vec{\nabla}_r + h \vec{\xi} \cdot \vec{\nabla}_p\right) \Theta = \Lambda + h T + o(h) .$$

The matrix $T$ describes the first-order contribution to the band-to-band transition, and will be evaluated in the following; $\Lambda\left(x, p, h \frac{\partial}{\partial x}, h \frac{\partial}{\partial p}\right)$ is a diagonal matrix of pseudo-differential operators (i.e., each element of $\Lambda$ is a differential operator admitting an $h$ expansion). Thus

$$\Lambda_{i,j}\left(x, p, \frac{\partial}{\partial x}, \frac{\partial}{\partial p}\right) = \delta_{ij}\left[h \left(\xi_i^\rightarrow \cdot \vec{\nabla}_r + \chi_i^\rightarrow \cdot \vec{\nabla}_p\right)\right] + o(h) .$$

We evaluate the matrix $\Theta$ in order to satisfy Eq. (8) up to the first order in $h$. We define by $u^k$ the column vector operator equal to the $k$-th column of $\Theta$ (i.e. $u_i^k = \Theta_{i,k}$ where the $i$ index denotes the $i$-th component of the vector $u^k$). We multiply Eq. (8) with $\Theta$ from the left and obtain

$$\left(A_0 + h \vec{B} \cdot \vec{\nabla}_r + h \vec{\xi} \cdot \vec{\nabla}_p\right) u^k = u^k \lambda^k + h \sum_j u^j T_{j,k}$$

where, according to the $h$ expansion of $\Theta$, $u^k$ is given by

$$u^k\left(x, p, \frac{\partial}{\partial x}\right) = u_0^k + h \vec{v}^k \cdot \vec{\nabla}_r + o(h) .$$

The zeroth order of Eq. (10) is

$$A_0(p) u_0^k = \lambda_0^k u_0^k$$

and we find that the $u_0^k$ are the eigenvectors of $A_0$. Here the $p$ variable is just a parameter. We calculate the first-order part of Eq. (10) by multiplying it from the left by $u_{0\dagger}^r$, where $\dagger$ denotes the algebraic conjugation. After some algebra we obtain

$$\vec{\chi}^k = \vec{\xi}$$

$$\vec{\xi}^k = (u_0^r, \vec{B} u_0^r)$$

$$T_{r,k} = \vec{\xi}^k \cdot (u_0^r, \vec{\nabla}_p u_0^k)$$

where $(,)$ denotes the ordinary scalar product $(a, b) = a^\dagger b$ and we expanded $v^k$ on the $u_0^k$ basis:

$$v^k = \sum_r -\frac{(u_0^k, \vec{B} u_0^r)}{(\lambda_0^k - \lambda_0^r)} u_0^r .$$
We consider the equation of motion for \( f' \equiv \Theta f \). By defining the components of \( f' \) as
\[
\begin{align*}
& f'(r, p) = \left( \begin{array}{c} f^+ \\ f^i \\ f^- \end{array} \right), \\
& \frac{\partial f'}{\partial t} = \pm v_F \frac{p}{|p|} \cdot \nabla_r f^\pm + \nabla_r U \cdot \nabla_p f^\pm \pm i \left( B f^i - \overline{B f^i} \right) \\
& \frac{\partial f^i}{\partial t} = i A f^i + \nabla_r U \cdot \nabla_p f^i + i \overline{B} (f^+ - f^-)
\end{align*}
\]
where overbar means conjugation and
\[
\begin{align*}
& A = -\frac{2v_F}{\hbar} \left( \frac{p}{|p|} + \frac{1}{|p|^2} (p \wedge \nabla_r U)_z \right) \\
& B = \frac{1}{2} \frac{p_x + ip_y}{|p|^3} (p \wedge \nabla_r U)_z.
\end{align*}
\]
Here \((p \wedge \nabla_r U)_z = \left( -\frac{\partial U}{\partial r_x} p_y + \frac{\partial U}{\partial r_y} p_x \right)\) denotes the out-of-plane component (\(z\)-coordinate) of the vector \((p \wedge \nabla_r U)\).

Despite the rather cumbersome derivation, Eqs. (12)-(13) provide a straightforward extension of the semi-classical particle-hole evolution equation in graphene. One of the principal aims of our diagonalization procedure was to derive a formalism where the free motion is easily described. As expected from a physical point of view, since the external field \(U(r)\) is the only perturbation to the periodic crystal potential, in the limit of a vanishing electric field, the equations decouple and the motion is described by two semi-classical equations. The density of particles and the current in the upper (lower) band, denoted by \( n^+ (n^-) \) and \( j^+ (j^-) \), respectively, can be obtained from the Wigner functions as
\[
\begin{align*}
& n^\pm(r, t) = \frac{1}{(2\pi \hbar)^2} \int f^\pm(r, p, t) \, dp \\
& j^\pm(r, t) = \pm \frac{ev_F}{(2\pi \hbar)^2} \int \frac{p}{|p|} f^\pm(r, p, t) \, dp.
\end{align*}
\]
The continuity equation for the charge can be derived from the system of Eqs. (12)-(13). We have
\[
\begin{align*}
\frac{\partial n^\pm}{\partial t} &= \nabla_r \cdot j^\pm + \int \mathcal{M}[f^i] \, dp \\
\mathcal{M}[f^i] &= \frac{1}{p^2} (p \wedge \nabla_r U)_z \Im \left\{ f^i e^{i\theta p} \right\}.
\end{align*}
\]
In particular for a stationary solution (where \( \frac{\partial n^{\pm}}{\partial t} = 0 \)) we have that \( \nabla_r \cdot j^t = 0 \), where \( j^t \) is the total current \( j^t \equiv j^+ + j^- \).

2.3. **Ballistic transport in intrinsic graphene.**

We apply Eqs. (12)-(13) to study the quantum correction to the ballistic charge motion in a graphene sheet in the presence of an applied external potential. In particular, we assume that the particles are accelerated by an external electric field directed along the \( x \) direction and independent of the \( y \) variable \( (\nabla_r U = \mathcal{E}(r_x) \hat{r}_x) \). In this case we can assume \( \frac{\partial f}{\partial r_y} = 0 \) which greatly reduces the numerical complexity of the system. The equations of motion become

\[
\begin{align*}
\frac{\partial f^\pm}{\partial t} &= \pm v_F \frac{p_x}{\sqrt{p_x^2 + p_y^2}} \frac{\partial f^\pm}{\partial x} + \mathcal{E} \frac{\partial f^\pm}{\partial p_x} \pm \mathcal{E} \frac{p_y}{p_x^2 + p_y^2} \left\{ \frac{p_x + ip_y}{\sqrt{p_x^2 + p_y^2}} f^i \right\}, \\
\frac{\partial f^i}{\partial t} &= iAf^i + \mathcal{E} \frac{\partial f^i}{\partial p_x} - \frac{i}{2} \mathcal{E} \frac{p_y}{(p_x^2 + p_y^2)^{3/2}} (f^+ - f^-),
\end{align*}
\]

where

\[
A = -\mathcal{E} \frac{p_y}{p_x^2 + p_y^2} - \frac{2v_F}{\hbar} \sqrt{p_x^2 + p_y^2},
\]

and \( \mathbf{p} = (p_x, p_y) \), \( \mathbf{r} = (x, y) \). We consider a simple device consisting of a graphene sheet suspended by two ohmic contacts at distance \( L = 1 \mu m \). The bias voltage \( U \) is applied between the contacts. This prototype of devices has been experimentally probed in Ref. [3]. The presence of interfacial phonons in the substrate revealed to be an important source of limitation for the charge mobility in graphene. However, suspended graphene offers the considerable advantage that the interactions between the underlying substrate and the graphene sheet are completely eliminated. Up-to-date lithographic technique allows the fabrication of high quality graphene sheets suspended on a silicon substrate of nearly 1 \( \mu m \) thickness. The mean distance between the flat graphene sheet and the substrate is around 150 \( nm \). At room temperature, mobilities of suspended graphene are closer to \( 10^4 \) \( \text{cm}^2\text{V}^{-1}\text{s}^{-1} \), and are limited by acoustic phonon scattering. Mobilities of such an order of magnitude imply that electrons can travel from one contact to the other by suffering only a few scattering events. This evidence justifies the study of ballistic transport in suspended graphene. In our model, we assume that the electric field is constant along the graphene sheet.
A direct solution of the system of Eqs. (20)-(21) and its application to electron transport in a graphene sheet encounters serious numerical difficulties. The main problem arises from the particular form of the equation of motion for the interband function \( f^i \). The diagonal functions \( f^{\pm} \) (which can be considered as a straightforward generalization of the distribution function of electrons in the upper and in the lower part of the Dirac cone) share similar properties with their classical counterparts, and are rather smooth and stable. On the contrary, the interband function \( f^i \) is a strongly oscillating function.

In order to illustrate the numerical problem in connection with a direct simulation of Eqs. (20)-(21), we plot a typical example of the solution in fig. 1. In particular, it displays the stationary solution \( f^i \) for a graphene sheet at the temperature \( T = 300 \) K in the presence of an applied voltage between source and drain of \( 0.3 \) eV. The numerical solution is obtained by using on some well established standard methods. Based on splitting algorithms, they are presented in Refs. [16]-[17], we used a discretization of the \( (x - p_z) \)
plane containing $N_x \times N_p$ points with $N_x = 200$ and $N_p = 200$. The solution shows the presence of several spikes which are clearly related to numerical noise. No considerable improvement is obtained by simply refining the mesh grid (the main features are still present and spikes appear randomly in the final result), which is, of course, not satisfactory.

2.4. Asymptotic procedure: numerical approach.

In this section, we propose an alternative strategy based on an asymptotic approach to overcome the problem of strong numerical noise observed when solving the Eqs. (20)-(21) directly. In the study of the electric properties in a solid, like the current-voltage (I-V) characteristic and the conductivity, it is often of primary interest to obtain a correct description of the non-equilibrium stationary state reached by the system in response to an external perturbation field. In the case of the I-V characteristic, the external perturbation is represented by the gradient of the applied potential. The knowledge of the stationary I-V characteristic is crucial for engineering applications of a material and to its integration in a network. In particular, a different behaviour of the considered problem is expected if it is characterized by a single time scale according to which all the interesting observables evolve, or if some observables evolve much faster than the others. In the latter case, these variables identify some “internal dynamics” of a multi-scale process. In our system, the interband function $f^i$ is a strongly oscillating function and its “natural” oscillation frequency $\omega$ depends on the momentum $p$. This reflects the general principle of quantum mechanics that a wave function containing a superposition of states with different energies, oscillates with a frequency which is proportional to this internal energy difference. In our case, $f^i(r, p)$ describes a mixture of states belonging to the upper and the lower cone. At a given position $r$, their mean energy difference is equal to $2v_F |p|$. This appears explicitly in Eq. (22) and, because of the high value of the Fermi velocity in graphene, this term induces a dynamical evolution of $f^i$ that can be considered considerably faster than the other processes induced by the external field (we remark that the identification of the different time scales in which the two-band quantum system evolves, is practically infeasible with the usual definition of many-band Wigner functions given in Eq. (3)). Since $f^\pm$ describe states with similar energy, in view of Eq. (20), no “natural” oscillation frequency is present in the equation for $f^\pm$.

In order to estimate the temporal evolution of the system of Eqs. (20)-(21), we consider a limit where the band-to-band transitions are not dominant, so that we can estimate the distribution $f^\pm$ as a perturbation of the
corresponding classical distribution functions. This is obtained in the limit of a small electric field $\mathcal{E}$. We formally expand the solution of Eqs. (20)-(21) in terms of the electric field $\mathcal{E}$. In the expansion $f^{\pm} = \sum_{n=0}^{\infty} f^{\pm}_n \mathcal{E}^n$, the zeroth-order approximation of the solutions $f^{\pm}_0$ are the classical distribution functions. Equation (21) for the interband function $f^i$ can be expressed in the integral form (we assume vanishing initial condition)

$$f^i(r, p, t) = \int_{t_0}^{t-t_0} e^{i \int_{t'}^{t} A(p_x + \mathcal{E} \tau) \, d\tau} \mathcal{D}(p_x + \mathcal{E} t') f^d(r; p_x + \mathcal{E} t', p_y; t - t') \, dt' \, ,$$

(23)

where we defined $f^d = f^+ - f^-$. The exponential term in Eq. (23) reveals the high-frequency oscillations of the function $f^i$. By inspecting Eq. (23), we observe that $f^i$ is of the first order in $\mathcal{E}$ (and vanishes in the limit of zero electric field). The long time-behaviour of the solution $f^i$ is dominated by the exponential term. In particular, since the momentum $p_x$ is evaluated along the trajectory $p_x(t) = p_x(t_0) + \mathcal{E}(t-t_0)$, the phase velocity $A$ changes in time and increases indefinitely for $t$ going to infinity. In view of the stationary phase approximation, a relevant contribution to the integral is provided only in the neighborhood of the minimum of the oscillation frequency (where $p_x(t') = 0$). The first non-vanishing contribution to the expansion $f^i = \sum_{n=0}^{\infty} f^i_n \mathcal{E}^n$, can be evaluated by approximating $f^d$ in Eq. (23) to the zeroth-order $f^d_0 = f^+_0 - f^-_0$, where $f^\pm_0 = (1 + e^{\pm v_F|p|})^{-1}$ are the Fermi distributions. By expanding $f^d$ around the stationary point $p_x = 0$, we obtain

$$f^d_0(r; p_x + \mathcal{E} t, p_y; t) \bigg|_{p_x = 0} \simeq \frac{t^2 v_F \mathcal{E}^2}{4 |p_y|} \, .$$

(24)

For a temperature $T = 300$ K, an electric field $\mathcal{E} = 0.1$ eV$\mu$m$^{-1}$ and a parallel momentum $p_y = 0.1$ nm$^{-1}$ (which are the typical values for graphene), the previous equation reveals that, around the stationary point $p_x = 0$, the $f^d$ function evolves in a time scale of picoseconds. This time scale is considerably smaller than the “natural” frequency $A$, which is of the order of femtoseconds. Furthermore, Eq. (24) shows that the time variation of $f^d$ is of the second-order in $\mathcal{E}$ and can thus be neglected. These considerations suggest to simplify the evolution of the system by assuming that the time variation of the diagonal functions $f^{\pm}$ is smooth compared to the time
Figure 2. Stationary values of the function $f^i$ in the presence of a uniform electric field $E$, obtained by using the recursive formula of Eq. (25) for different values of the momentum $p_y$. Left panel $p_y/\hbar = 0.4$ nm$^{-1}$, right panel $p_y/\hbar = 2 \cdot 10^{-3}$ nm$^{-1}$.

The evolution of $f^i$. In this hypothesis, we consider an asymptotic model where the function $f^d$ is assumed to be constant around the stationary point $p_x = 0$. Furthermore, we integrate out the fast-in-time dynamics of $f^i$ by letting $t$ go to infinity in Eq. (23). In order to obtain an efficient integration scheme for Eq. (23), it is convenient to define

$$F^i(p_x,t) \equiv \int_{0}^{t-t_0} D(p_x + E \tau') e^{i \int_{0}^{\tau'} A(p_x + E \tau') \, d\tau'} \, d\tau'.$$

We then obtain

$$F^i(p'_x,t) = e^{-i \int_{0}^{t} A(p_x + E \tau) \, d\tau} \left[ F^i(p_x,t + \tilde{t}) - F^i(p_x,\tilde{t} + t_0) \right],$$

where $p'_x = p_x + E \tilde{t}$. In case that $f^d$ is nearly constant, we use the approximation

$$f^i \approx f^d(r,p) \lim_{t \to \infty} F^i.$$

The recursion formula, Eq. (25), is particularly useful to get a high-precision approximation of the function $f^i$. In this way, instead of calculating the integral of Eq. (23) directly, (where we need to compute the integral along the full time interval from $t_0$ to infinity), and repeating this calculation for each values of the momentum $p_x$ (which now plays the role of a parameter), by using Eq. (25), we obtain the values of the function at the grid points $p'_j = p_0 + j E \Delta \tilde{t}$ only by evaluating the integral over the interval $\Delta \tilde{t}$. In fig. 2 we display the interband function $f^i$ obtained by using Eqs. (25)-(26) for the same parameters as in fig. 1. The plot shows that, as expected, the function $f^i$ displays high-frequency oscillations along the $p_x$ axis. This
behaviour becomes more and more evident when the parallel momentum \( p_y \) goes to zero. A resolution of nearly \( 10^5 \) points in the \( p_x \) axis is required, for \( p_y/\hbar \) to be of the order of \( 10^{-3} \) nm\(^{-1} \). In graphene, the band-to-band transition probability approaches to one for \( p_y = 0 \). For this reason, small values of \( p_y \) characterize the interesting regime, when we study quantum corrections to the interband current. Moreover, Eq. (22) shows that for \( p_y \) going to zero, the function \( f^i \) oscillates with a period of \( \Delta p_x \propto \hbar E/v_F \). The increase of the oscillation frequency along the \( p_x \) axis, when \( p_x \) increases (we recall that the electric field is directed along the \( x \) axis and we are evaluating the integral along the trajectory \( p_x(t) = p_x(t_0) + \mathcal{E}(t - t_0) \)), makes the direct numerical approximation of \( f^i \) impracticable and explains the important numerical errors encountered by a direct discretization of the system of Eqs. (12)-(13). Finally, we note that the high oscillating behaviour of \( f^i \) contrasts the form of the diagonal functions \( f^\pm \) that stay smooth even in the presence of significant band-to-band transitions. Thus it ensures the validity of the approximation used in Eq. (26).

2.5. Asymptotic procedure: closed-form approximation.

Based on the approximations described in sec. 2.5, we derive a closed analytic solution for the interband function \( f^i \). It is convenient to write Eq. (23) as

\[
 f^i(r, p, t) = \int_{t_0}^{t} e^{i \int_{t'}^t A(\mathcal{T}(t-\tau)p) \, d\tau} \mathfrak{F}(t, t') \, dt',
\]

where

\[
 \mathfrak{F}(t, t') = \mathcal{D}(\mathcal{T}(t-t')p)f^d(r, \mathcal{T}(t-t')p, t')
\]

and \( \mathcal{T}(t)p \equiv p_x(t) = p_x + \mathcal{E}t \) is the trajectory of a particle with momentum \( p \) accelerated by a uniform electric field \( \mathcal{E} \). In the spirit of the stationary phase approximation, we expand the function \( A \) around \( t^* = p_x/\mathcal{E} \) and the integral simplifies to

\[
 f^i \approx -\frac{e^{i g_0(t^*)^3}}{\sqrt{8\pi}} \int_{-t^*}^t e^{-i \left( \frac{g_0}{\sqrt{8\pi}} \tau + \frac{3}{8} \right)} \mathfrak{F} \left( t, t - t^* - \frac{\tau}{\sqrt{8\pi}} \right) \, d\tau
\]

where

\[
 g_0 = A(\mathcal{T}(t^*)p) = -\frac{\mathcal{E}}{p_y} - \frac{2v_F}{\hbar} |p_y|,
\]

\[
 g_2 = \frac{1}{2} \left. \frac{d^2 A(\mathcal{T}(u)p)}{du^2} \right|_{u=t^*} = -\mathcal{E}^2 \left( \frac{1}{p_y^2} \mathcal{E} + \frac{v_F}{\hbar |p_y|} \right).
\]
To evaluate the integral, we simply assume that the function $\mathcal{F}$ is nearly constant with respect to the time scale $1/\sqrt{g_2}$. By noting that $\mathcal{F}(t, t - t^*) = \mathcal{D}(T(t^*)p)f^d(T(t^*)p, t - t^*) = \mathcal{D}(T(t^*)p)f^d(p, t)$, we obtain

$$f^i \simeq -\frac{\pi E}{p_y \sqrt{g_2}} \text{Ai}\left(\frac{g_0}{\sqrt{g_2}}\right) \theta(p_x E) e^{i\left(\frac{(g_x t^*)^3}{3} + g_0\right)} f^d(x, t),$$

where $\theta$ denotes the Heaviside step function and $\text{Ai}(x)$ is the Airy function:

$$2\pi \frac{\text{Ai}\left(\frac{a}{\sqrt{b}}\right)}{\sqrt{b}} = \int_{-\infty}^{\infty} e^{i(a t + \frac{b}{3} t^3)} \, dt.$$

2.5.1. Simulation of graphene.

![Graphene simulation snapshots](image-url)

Figure 3. Stationary solution for graphene for an applied potential $V_0 = 0.3$ eV. Snapshots of the $f^+$ (upper plot), $1 - f^-$ (lower plot) distributions on the $(x - p_x)$ plane, for $p_y/h = 0.1 \text{ nm}^{-1}$. In the left plot we represent the contour lines and in the right plot the 3D representation of the solutions.

We apply our asymptotic model, constituted by Eqs. (20)-(26), to obtain quantum corrections to the stationary current induced by the Klein tunneling. We prescribe boundary conditions in correspondence to the metallic
contacts. The contacts are considered as perfect charge reservoirs, where the number of particles entering in the device (with positive velocity in the left contact and negative in the right contact) are given by the thermal equilibrium distribution. By identifying $f^+$ and $f^-$ with the electron distribution functions in the upper ($\Sigma^+$) and lower ($\Sigma^-$) cone, respectively, we
fix their incoming values at the boundary of the simulation domain equal to the Fermi distribution function. Vanishing boundary conditions are assigned to the interband function $f^i$. In our simulation, we assume $L = 1 \mu m$ and the lattice temperature $T = 300$ K.

In the Figures 3-4 we depict the stationary values of the electron conduction distribution $f^+$ and the valence hole distribution $1 - f^-$ for an external applied potential $V_{ext} = 0.3$ eV for different values of the orthogonal momentum $p_y$. In the left plots we represent the contour lines and in the right plots the 3D representation of the solutions. It can be clearly seen that the electrons split in two parts: the particles with velocities parallel to the electric field which are accelerated, and anti-parallel ones which are reflected back by the potential barrier. Further, due to the presence of interband Klein tunneling, also interband particle transition between the bands $\Sigma^+$ and $\Sigma^-$ are possible. Since the relation between the velocity and the momentum for a hole is the inverse of that for an electron during this interband transition, the momentum parallel to the barrier is conserved and the velocity of the quasiparticle is inverted. Due to the larger number of particles in the lower cone, we observe a net flux of particles from $\Sigma^-$ towards $\Sigma^+$. As expected, interband transitions become a dominant phenomenon around $p = 0$. For this reason, in correspondence to high values of $p_y$ (plots of Figure 3), the distribution functions look very similar to their classical counterparts and quantum corrections are negligible. On the contrary, for smaller values of $p_y$ (plot 4) a flux of particles from the $\Sigma^-$ band to the $\Sigma^+$ band is clearly visible. To highlight the effect of the Klein tunneling, in Figure 4-e-f we report the distribution functions of electrons and holes under the same condition as in Figure 4-a-b but in the semi-classical approximation (without tunneling). From Figure 4-a (right panel) we see that a large number of particles coming from the source contact $x = -L$, which are decelerated by the electric field in order to overcome the linear potential barriers, leave the $\Sigma^-$ band (this leads to an increasing of the hole distribution function $1 - f^-$). These particles are now accelerated by the same electric field in the final part of the device ($x = L$) and contribute to increase the particle distribution $f^+$.  

3. Conclusion.

In this contribution, the ballistic transport of electrons in graphene by including quantum effects is investigated in terms of the Wigner formalism. The resulting formulation reveals to be particularly close to the classical description of the particle motion. Special attention is devoted to model the Klein tunneling and to study the correction to the total current in
intrinsic graphene induced by this phenomenon. Due to the high numerical complexity of the resulting system of equations, an approximate closed-form solution is obtained. The simulations show that for an intrinsic graphene in the presence of a strong electric field, our model predicts a non-negligible correction to the charge inside the device.

Acknowledgements.

This work has been supported by the Austrian Science Fund, Vienna, under the contract No. P 21326 - N 16.

REFERENCES


