Geometrically induced rectification in two-dimensional ballistic nanodevices

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Abstract
This paper demonstrates that a two-dimensional ballistic nanodevice in which the electron gas satisfies either the Schrödinger equation (as in quantum wells in common semiconductor heterostructures) or the Dirac equation (as in graphene) is able to rectify an electric signal if the device has a non-uniform cross-section, for instance a tapered configuration. No p–n junctions or dissimilar electrodes are necessary for rectification.

1. Introduction
The process of rectification transforms a signal in alternating current (ac) to a direct current (dc) one. Rectification is a key signal processing tool in many applications, ranging from power supplies up to high-frequency detectors, and is present in smart phones, computers, TV sets and radio wireless communication. Rectification is implemented using a semiconducting p–n junction obtained by chemical doping. However, in two-dimensional electron gas (2DEG) devices based on semiconducting heterostructures or graphene, chemical doping becomes difficult and is replaced by electrostatic doping performed by multiple metallic gate electrodes biased by means of different dc voltages [1–3]. Also, in carbon nanotubes rectification can be achieved by Schottky contacts implemented with the help of dissimilar or asymmetric electrodes made from different metals [4, 5]. However, metallic gates on nanostructures complicate the architecture of rectifying devices considerably, using extensive nanolithography techniques, and quite often introducing parasitic effects in rectifying nanodevices.

Therefore, it is very important to rectify ac signals by means of a mechanism different with respect to chemical doping or Schottky contacts. Tailoring the shape of semiconductor channels was used already in self-switching devices, but was not related to ballistic transport [6], whereas a unipolar diode working as room-temperature THz detector based on symmetry breaking of a semiconducting channel was demonstrated recently [7]. Geometrical asymmetries are used in non-ballistic metal–insulator–metal diodes to enhance the sensitivity of electromagnetic wave detection at 900 MHz, which remains, however, quite low [8].

A typical 2DEG ballistic rectifier consists of a triangular-shaped scatter placed in the middle of a channel terminated with two contacts defined as drain (D) and source (S) [9]. This type of rectifier can work in the frequency range 50–110 GHz, but has poor responsivity because of the very large mismatch between the impedance of the rectifier and the standard 50 Ω of any high-frequency equipment [10]. Only 0.4% of the excitation power reaches the rectifier [11]! To alleviate this drawback we propose a tapered rectifier with a trapezoidal shape, based on the fact that a taper is the optimal geometry for matching the impedance of an incoming electromagnetic field.

Hence, the aim of this paper is to investigate the rectifying properties of a 2DEG nanodevice with a linear tapered geometry working in the ballistic regime, where the transport of charge carriers is described by either the Schrödinger or the Dirac equation. We show that such a device can rectify ac electrical signals under certain conditions, at room temperature, thus paving the way for the generation of THz signals via multiplication and for the detection of THz signals used in imaging applications.
A diagram showing a schematic representation of a linear tapered 2DEG connected at two metallic electrodes is displayed in figure 1; we assume throughout this paper that $d_{\text{in}} > d_{\text{out}}$. Rectification occurs for current flowing along the x direction. We assume that the boundaries of the linear tapered 2DEG act as regions with an infinite energy potential and model the transport of charge carriers by replacing the linear taper with a number of $N$ regions with constant but different widths, shown as rectangles with dotted boundaries in figure 1. In each region of width $d_j$, $j = \text{in}, 1, \ldots, N, \text{out}$, the wavevector component along $y$ has discrete values $n\pi/d_j$, so that the wavevector component along $x$ is equal to $k_{n,j} = \sqrt{2m(E - V_j)/\hbar^2} - (n\pi/d_j)^2$, where $m$ and $E$ are the effective mass and energy of the electron, respectively, and $V_j$ is the potential energy in region $j$. A solution of the Schrödinger equation in region $j$ since tunnelling has no role at each interface between different regions $N$. The voltage dependence of the transmission coefficient $T$ was discretized. Therefore, the transmission probability is determined by the requirement of flux conservation:

$$T = \frac{\sum_{n=1}^{N_{\text{in}}} k_{n,\text{out}} |A_{n,\text{out}}|^2}{\sum_{n=1}^{N_{\text{in}}} k_{n,\text{in}} |A_{n,\text{in}}|^2},$$

where the coefficients $A_{n,j}$ represent the amplitudes of the forward-propagating components of the wavefunction in the incidence and outgoing media, respectively, and are found by imposing the continuity conditions for the solutions

$$\Psi_j(x, y) = \sum_{n=1}^{N_j} \left[ A_{n,j} \exp(i k_{n,j} x) + B_{n,j} \exp(-i k_{n,j} x) \right] \sin(2n\pi y/d_j)$$

of the Schrödinger equation in region $j$ and its derivative with respect to $x$ at each interface between different regions (for details on electron propagation in waveguides with non-uniform cross-section, see [12, 13]).

The voltage dependence of the transmission coefficient for $E = 0.2$ eV is represented in figure 3 for the case of a step interface between the incoming and outgoing media, i.e. for
of the Fermi energy level: $E_F$, the Landauer formula, is represented in figure 4 for three values of $N$: $N = 0$ (red dotted line), and for $N = 1$ (black solid line) and $N = 2$ (blue dashed line). As $N$ increases, the transmission coefficient resembles the smooth curve represented with the green dashed–dotted line in figure 3. From this figure it follows that, because the number of modes depends on the polarity of the applied voltage (see figure 2), the transmission through the tapered configuration also depends asymmetrically on $V$: it takes high values for positive biases and low values for negative biases, indicating no current transport for which there are no propagating outgoing modes. As suggested by figure 2, the bias voltage for which $T$ increases sharply increases as the energy decreases.

The current at room temperature, calculated with the Landauer formula, is represented in figure 4 for three values of the Fermi energy level: $E_F = 0$ (blue dashed line), 0.1 eV (black solid line) and 0.2 eV (red dotted line). Although current rectification occurs in all the cases, the shape of the $I–V$ characteristic depends on the position of the Fermi level. A low $E_F$ corresponds to lower energy values of the charge carrying electrons, for which $T$ can have significant values for only one polarity (see the blue dashed line), while for high enough Fermi levels the transmission probability has a finite value at $V = 0$ (see also figure 3), so that current flows also for a limited range of negative $V$ values. Therefore, to have current flow only for one polarization, one must choose $E_F$ appropriately.

The rectifying behaviour is determined mainly by the value of $d_{out}$. To illustrate this fact, we have represented in figure 5(a) the current–voltage characteristics for $E_F = 0$ and $d_{in} = 50$ nm, $d_{out} = 10$ nm (black solid line), $d_{in} = 100$ nm, $d_{out} = 10$ nm (blue dashed line) and $d_{in} = 100$ nm, $d_{out} = 20$ nm (red dotted line). As $d_{in}$ (the tapering angle) increases with respect to $d_{out}$ the transmission coefficient and hence the current decrease due to an increased mismatch between the incidence and outgoing regions. However, the overall shape of the current–voltage characteristic remains the same. On the other hand, although the black solid and red dotted curves in figure 5(a) correspond to the same tapering angles, the $I–V$ characteristic differs since the number of outgoing modes for a given $V$ increases for the red dotted curve because $d_{out}$ is larger, and there is a finite number of outgoing modes for $V = 0$. As a consequence, a negative bias must be applied to have $N_{out} = 0$, which explains the existence of a negative current in a narrow negative voltage region for the red dotted curve in figure 5(a).

This explanation is supported by figure 5(b), which shows the dependence on $V$ of the ratio of outgoing and incoming mode numbers for the three cases studied in figure 5(a) with the same line type for $E_F = 0$ and $T = 300$ K the room temperature.

### 3. Signal rectification by a tapered graphene sheet

Graphene is a natural 2DEG, in which the charge carriers satisfy a massless Dirac equation. As a result, an infinite graphene sheet has no bandgap, although a finite bandgap exists in narrow graphene strips, also called nanoribbons. Because of the spatial confinement of the spinorial wavefunction in our linear tapered configuration, there is a small bandgap with a linearly varying width, which increases towards the outgoing region.

The mathematical treatment of the graphene taper parallels that of the previous section. In particular, the linear taper is again modelled as a succession of $N$ regions with widths $d_j$, $j = 1, \ldots, N$, out, so that the wavevector component along $y$ is again discrete and given by the same expression as in the previous section, the wavenumbers along $x$ being now $k_{n,j} = \text{sgn}(E - V_j)\sqrt{(E - V_j)^2/(\hbar^2v_F^2) - (n\pi/d_j)^2}$ [14], where $v_F \equiv c/300 \ldots$
is the Fermi velocity. If $\text{sgn}(E - V_j)$ is positive the electrical charge is carried by electrons, otherwise it is carried by holes. In the tapered waveguide charge propagation occurs for real $k_{n,j}$ values, the number of modes in the $j$th region being now given by $N_j = \text{Int}[d_j|E - V_j|/(\pi \hbar v_F)]$. The expressions of $d_j$ and $V_j$ are the same as in the previous case.

In the graphene taper, with $d_{in} = 50 \text{ nm}$, $d_{out} = 10 \text{ nm}$, the voltage dependence of the ratio of outgoing and incoming mode numbers is represented in figure 6 for $E = 0.1 \text{ eV}$ (blue dashed line), 0.2 eV (solid black line) and 0.3 eV (red dotted line). These curves are independent of the number of discretization regions $N$. Although there are a finite number of outgoing modes for both voltage polarizations, in all cases there is a voltage range in which no charge carriers are transmitted since for these $V$ values the number of outgoing modes, and hence the current, vanishes. This region, with a width given by $\pi \hbar v_F/d_{out}$ can be exploited to achieve current rectification. The width of the region increases as $d_{out}$ decreases. Please note that the voltage range in which $N_{out} = 0$ does not depend on the energy of the incident electrons, but shifts to lower values as the energy increases.

The transmission coefficient is now defined as

$$T = \sum_{n=1}^{N_{in}} |A_{n, out}|^2 / \sum_{n=1}^{N_{in}} |A_{n, in}|^2,$$

(3)

where the coefficients $A_{n,j} = \text{in, out}$ are calculated by imposing the continuity conditions at each interface for the spinorial solutions of the Dirac equation in region $j$:

$$\Psi_j(x, y) = \begin{cases} \sum_{n=1}^{N_j} [A_{n,j} \exp(i k_{n,j} x)] \sin(2n\pi y/d_j) + B_{n,j} \exp(-i k_{n,j} x)] \sin(2n\pi y/d_j) \quad \text{if} \quad x < 0 \\ \sum_{n=1}^{N_j} [A_{n,j} \exp(i k_{n,j} x)] \sin(2n\pi y/d_j) - B_{n,j} \exp(-i k_{n,j} x)] \sin(2n\pi y/d_j) \quad \text{if} \quad x > d_j \end{cases}$$

(4)

Figure 7 shows the transmission coefficient dependence on $V$ for $E = 0.2 \text{ eV}$ and for $N = 0$ (red dotted line), $N = 1$ (black solid line) and $N = 2$ (blue dashed line). $T$ tends to the green dashed–dotted line for large $N$ values. Unlike for Schrödinger-type charge carriers, the transmission has significant values for both bias polarizations, except for a narrow voltage range in which there are no outgoing modes.

The current through the tapered graphene, calculated also with the Landauer formula, is represented in figure 8 for three values of the Fermi energy level: $E_F = 0$ (blue dashed line), 0.1 eV (black solid line) and 0.2 eV (red dotted line). As follows from figure 8, the shape of the $I–V$ characteristics is the same in all cases, but the current amplitude depends on the Fermi level (on the energy of electrons that contribute to the current flow). Unlike for Schrödinger-type charge carriers, the $I–V$ characteristics are symmetric around a bias voltage that represents the centre of the region in which the transmission coefficient/number of outgoing modes vanishes. Current rectification can occur only if the Fermi level is chosen such that the sudden current increase or decrease takes place at $V = 0$. Such a situation is represented with the red dotted line in figure 8. In this case current rectification, in the sense that finite current values exist for one polarization only, occurs if the incident voltage signal has an amplitude (in this

Figure 6. Voltage dependence of the ratio of outgoing and incoming mode numbers in graphene for $E = 0.1 \text{ eV}$ (green dashed line), 0.2 eV (solid black line) and 0.3 eV (red dotted line).

Figure 7. Voltage dependence of the transmission coefficient in graphene for $E = 0.2 \text{ eV}$ and for $N = 0$ (red dotted line), 1 (solid black line) and 2 (green dashed line). $T$ tends to the magenta dashed–dotted line for large $N$ values.

Figure 8. Current–voltage characteristics in graphene for $E_F = 0$ (green dashed line), 0.1 eV (solid black line) and 0.2 eV (red dotted line).
on a doped Si/SiO2 substrate and coupled to a bowtie metallic line), numbers for E characteristics depend mainly on the rectified if section). Voltage signals with higher amplitudes could be amplitude of electrical signals (see the results in the previous simulation) lower than 0.4 V. Note that current rectification properties of this diode are relatively poor and its nonlinearities are very weak even at gate voltages of 40 V. These poor results are caused by the high losses of the doped Si substrate, which appear even beyond a few GHz [16], and by the non-ballistic transport of charge carriers, the length of the device being 1 µm. At room temperature, the ballistic transport in graphene occurs for a mean-free path of 0.4 µm, reaching an intrinsic mobility of 44 000 cm2 V−1 s−1 [17], mean-free carrier paths longer than 1 µm and mobilities higher than 100 000 cm2 V−1 s−1 being observed only in the exceptional case when graphene is deposited on a hexagonal boron nitride substrate [18] matching the graphene lattice. However, the ambipolar character of the rectification predicted in this paper was experimentally observed in [15].

4. Cutoff frequency of the rectifier

The cutoff frequency of our device can be written as

\[ f_c = \frac{v_p}{2\pi L}, \]  

where the propagating velocity of charge carriers \( v_p \) is equal to the Fermi velocity \( v_F \) for the Fermi velocity in graphene, with \( c \) the speed of light in vacuum. From equation (5) it follows that \( f_c = 1.6 \text{THz} \) for \( L = 100 \text{nm} \), while for \( L = 50 \text{nm} \) the cutoff frequency of the device reaches 3.2 THz. In quantum wells, in which electrons satisfy the Schrödinger equation, the propagating velocity is slightly lower than the Fermi velocity in graphene, but there are heterostructures such as InAs/AlSb, where the electron velocity is \( 10^8 \text{cm s}^{-1} \) at room temperature [19], equal to the Fermi velocity in graphene. Therefore, we can say that in the case of quantum well rectifiers the cutoff frequency \( f_c \) could also attain the THz range.

5. Conclusions

We have demonstrated that rectification, which is a key electronic function, takes place in two-dimensional ballistic nanodevices, in which the electron gas is described by either the Schrödinger equation or the Dirac equation, only when the 2DEG geometry is asymmetric with respect to the current flow direction. While in quantum wells described by Schrödinger equation the rectification is produced for a single, positive polarity of the electrical field (or negative polarity in two-dimensional hole gases), in the case of graphene, which fulfils a Dirac-like equation, rectification is ambipolar. Ambipolarity is an imprint of all graphene devices. Although our simulations were carried out for linear tapers only, the current rectification mechanism is the same in an arbitrarily shaped ballistic structure in which \( d_{in} > d_{out} \), so that it could be observed in any asymmetric device.

Because the cutoff frequencies of the above devices are located in the THz region, our results open up the perspective of generating THz frequencies, using multipliers with a much simpler architecture, and of imaging THz radiation by connecting the above rectifiers with small antennas on a single Si wafer. These applications are valid either for quantum well rectifiers described by the Schrödinger equation or for graphene rectifiers described by the Dirac equation. While
in the case of graphene the applications are potentially useful for THz imaging, the rectifier based on trapezoidal quantum wells can be used as a THz detector if connected to an antenna. Although the configuration of such a rectifier would be similar to the non-ballistic device in [7], a ballistic rectifier would have a significantly reduced noise and better overall performances of the THz receiver at room temperature.

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