Numerical simulation of the transport behavior of a graphene $p$-$n$-$p$ structure

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Abstract: - We describe a numerical method suitable to understand transport in graphene $p$-$n$-$p$ structures. Our approach is based on a simplified electrostatic model and on an envelope-function based transport code. In particular, we have been able to model Fabry-Pérot resonances in the potential cavity defined by the double junction and to reproduce existing data of scanning gate conductance spectroscopy.

Key-Words: - numerical simulation, graphene, junctions, electrostatics, transport, Dirac equation, scanning probe conductance spectroscopy, Fabry-Pérot resonances

1 Introduction
Graphene is a material that is receiving a lot of attention [1-8], due to its physical peculiarities and to its electrical, optical, mechanical and thermal properties, which make it interesting both for research and for industrial applications.

In particular, a large effort is focusing on a possible use of graphene in the fabrication of nanoelectronic devices [9,10]. Graphene-based electronic devices have been proposed, for example, for digital [11,12] and radiofrequency [13] applications and for the fabrication of sensors [14,15].

Recently a “charge writing” technique, which can be adopted for the fabrication of graphene-based devices, has been applied to pattern the potential landscape of nanodevices [16]. For graphene, in particular, a dielectric PMMA (polymethyl methacrylate) layer is deposited over the flake and charge is injected into it by means of a scanning probe, thereby altering the charge density in the graphene flake. In particular, in Ref. [17] a line of positive charge is deposited into the PMMA layer, thus defining a $p$-$n$-$p$ structure in the underlying graphene sheet, which is then investigated by means of resistance and scanning gate conductance spectroscopy measurements.

Here we describe a numerical method that we have developed to reproduce the experimental results of Ref. [17], and the outcome of some simulations.

2 Mathematical method
In order to perform simulations for a wide range of bias voltages and for several choices of potential profiles in a reasonable time, we have adopted an approximate but efficient method for the determination of the electrostatic landscape. Moreover, since we have been interested in the simulation of a graphene flake a few micron wide and thus containing several thousands of carbon atoms, we have used an envelope function ($k\cdot p$) description for the flake, instead of performing a full atomistic simulation.

2.1 Electrostatic simulation
In principle, an exact simulation of the device would require a self-consistent solution of the electrostatic and transport equations. In order to speed up our analysis, we have adopted a more simplified and approximate approach, bypassing this self-consistent calculation under the hypothesis of a slow-varying potential profile and substituting the solution of the Poisson equation with a simple capacitive model for the device [18].

We have assumed to know the potential profile $U_0(r)$ in every point $r$ of the flake for a given set of gate bias voltages $V_{G\theta}$ and we have then evaluated its variation as the $V_{G\theta}$ voltages are changed.

In detail, if the voltages applied to the gates vary by $\Delta V_{G\theta}$ with respect to the reference values $V_{G\theta}$ they induce a change $\Delta \rho$ in the graphene charge density $\rho$ (with respect to the charge density $\rho_0$ which exists when the gates are biased at $V_{G\theta}$). Due to the finite density of states of graphene, this corresponds to a shift $\Delta U$ of the graphene potential $U$ with respect to $U_0$. In particular, the charge density $\rho(r)$ is related to the potential energy $U(r)$ through the local density of states $LDOS(E,r)$ (where $E$ is the energy). The exact local density of...
states depends on the value of the wave function and thus would require the solution of the transport equation. However, under the hypothesis of slowly variable potential, we can approximate it with the density of states shifted by the local value of the potential \( U \): \( \rho \cdot DOS(E) = DOS(E-U) \). Therefore, under the further hypotheses of quasi-equilibrium and low-temperature operation, we have that

\[
\rho_o + \Delta \rho = e \int_{E_F}^{E_F+\Delta U} DOS(E-U_o-\Delta U) dE
\]

\[
= \text{sign}(U_o + \Delta U - E_F) \frac{e(U_o + \Delta U - E_F)^2}{\pi \hbar v_F^2},
\]

where \( e \) is the elementary charge, \( E_F \) is the Fermi level (determined by the contacts) and in the last step we have exploited the expression of the density of states in monolayer graphene.

Moreover, the relation between the charge in the device and the voltages on the bias gates can be schematically modeled through the electrostatic capacitances (per unit area) \( C_G(r) \) which couple the gates to each point \( r \) of the graphene layer:

\[
\Delta \rho = \sum_i C_G (\frac{\Delta U}{-e} - \Delta V_G). \tag{2}
\]

Substituting Eq. (2) into Eq. (1) we obtain a second-order equation that can be analytically solved, obtaining the value of \( \Delta U \). This calculation has been repeated for all the points \( r \) of the flake, in such a way as to obtain the profile \( U(r) \) in the device.

### 2.2 Transport simulation

Then the potential profile \( U(r) \) has been used to compute the conductance of the sample. In order to achieve this result, we have used our envelope-function based transport code for graphene armchair ribbons [19,20], based on the solution of the Dirac equation (which represents the envelope-function transport equation for monolayer graphene [21]) in the device.

In analogy with what we have previously done for the numerical analysis of GaAs/AlGaAs based devices [22-27], in our simulations we have subdivided the ribbon into a series of sections within each of which the potential energy is approximately constant in the transport direction. In each of these sections, the analytical system represented by the Dirac equation with the proper boundary conditions, i.e. the vanishing of the wave function at the edges of the flake, has been recast into an equivalent differential problem with periodic boundary conditions [19,28], that has been very efficiently solved in the reciprocal space.

Once we have computed the eigenfunctions in all the sections, we have enforced the continuity of the wave function along the interface between each pair of adjacent sections, obtaining the scattering matrix which relates the modes in the two sections. Iteratively composing the scattering matrices of all the regions of the device, we have obtained the scattering matrix from the entrance to the exit of the graphene ribbon and thus, as a submatrix, the overall transmission matrix \( t \).

Finally, the conductance \( G \) of the sample has been computed from \( t \) using the Landauer-Büttiker formula.

### 3 Numerical results

We have considered a 2.5 \( \mu \)m wide and 1\( \mu \)m long armchair ribbon. The Fermi energy has been set at the value \( E_F=0 \). For the capacitance (per unit area) which couples the backgate to the graphene flake we have assumed a value \( C_{BG}=0.1151 \text{ mF/m}^2 \). In the transport calculation we have divided the overall flake into 4 nm long sections and we have considered 330 modes.

![Fig. 1 Longitudinal section of the potential profile that best fits the experimental results, reported for three different values of the voltage \( V_{BG} \) applied to the backgate.](image)

In order to understand the shape of the electrostatically induced cavity of Ref. [17], we have tried to achieve the best agreement between our numerical transport results and the experimental measurement of resistance as a function of the voltage \( V_{BG} \) applied to the backgate. While for low (high) values of \( V_{BG} \) the cavity-shaped potential profile is everywhere over (under) the Fermi energy and does not have a significant effect on transport, for intermediate values of \( V_{BG} \) Fabry-Pérot resonances appear in the behavior of the resistance as a function of \( V_{BG} \) [29].

We have tested several cavity shapes, widths and depths in order to reproduce the positions of the experimentally measured Fabry-Pérot resonances. We have found the best fit considering for the reference backgate voltage \( V_{BG}=0 \) the Lorentzian profile \( U_0=\frac{a-b}{1+(\frac{x-x_0}{c})^2} \), with \( a=125 \text{ meV}, b=210 \text{ meV}, c=90 \text{ nm} \) and \( x_0 \) the coordinate at the center of the cavity. In Fig. 1 we represent a longitudinal section of the profile at \( V_{BG}=0 \), together with the corresponding profiles for \( V_{BG}=-10 \text{ V} \) and for \( V_{BG}=10 \text{ V} \), obtained with our simplified electrostatic calculation. In Fig. 2 we report with dotted lines the corresponding behavior of the resistance as a function of \( V_{BG} \). In the experimental data the presence of potential disorder, resulting from randomly located charges and impurities, increases the overall value of the resistance and superimposes random aperiodic fluctuations on the effects deriving from interference. However, our
numerical simulations clearly capture the main features of the resistance behavior. In particular, the values of $V_{BG}$ for which the Fabry-Pérot maxima appear are in very good agreement with the experimentally measured results.

Fig. 2 Behavior of the resistance as a function of the backgate voltage, obtained neglecting (dotted curves) or considering (solid curves) the effect of the division into subcavities and of the electric field focusing at the edges of the flake.

We have then simulated the scanning probe conductance spectroscopy experiment, in which a negatively biased probe is scanned over the graphene sample. For each position of the probe the resistance of the sample, affected by the probe, is computed. Finally a two-dimensional map of the measured resistance values as a function of the probe position can be created. We have included the effect of the biased probe through a spatially variable capacitance, with a Lorentzian dependence on the distance between the projection on the flake of the tip apex and the considered point of the graphene flake, assuming a maximum capacitance of $0.1171 \text{ mF/m}^2$ and a half-width at half-maximum of 50 nm. Comparing our results with the measured data reported in Ref. [17], we have concluded that the actual cavity is made up of 3 cavities in parallel, with different depths and widths. In particular, a very good fit has been obtained considering an average distance between the centers of adjacent cavities equal to 1 $\mu$m and a height of the separation walls equal to 1/10 of the cavity depths. A further improvement has been obtained including in our model the deviation from the bulk profile that has been previously observed at the edges of graphene flakes. In particular, on the basis of an analytical calculation, Ref. [30] reports a strong increase of the electric field, and a corresponding accumulation of mobile charges, at the edges of the graphene layer. We have included this effect properly modulating the potential profiles as a function of the distance from the edges. In Fig. 3 we show a map of the resulting potential profile for $V_{BG}=0$.

Fig. 3 Map of the potential profile in the flake for $V_{BG}=0$, including the division into subcavities and the field focusing effect at the edges.

The biased probe, perturbing the graphene potential profile, alters the scattering experienced by the mobile charges inside the flake and in particular modifies the interference pattern inside the sample, shifting the values of $V_{BG}$ for which the Fabry-Pérot resonances take place. This gives rise to the circular halos which appear in Fig. 4, where we report the resistance map obtained from the simulation of a scanning probe conductance spectroscopy experiment.

Fig. 4 Map of the resistance of the flake (obtained from our numerical simulations), reported as a function of the position of a biased probe kept at a fixed distance over the graphene sheet.

In order to better understand the effect of the potential details on the transport characteristic of the device, we have repeated the calculation of the resistance as a function of $V_{BG}$ considering also the division into subcavities and the edge effect that we have not included in the results reported with dotted lines in Fig. 2. We have observed that the division into subcavities partially suppresses the Fabry-Pérot resonances, that however still clearly appear. Numerical simulations show that the inclusion of the electric field focusing effect instead introduces further resonances in the resistance behavior, with a smaller amplitude and period. As suggested in Ref. [17], this effect could be attributed to the presence of a larger capacitive coupling
between the backgate and the flake at the edges of the ribbon. The curves obtained from our numerical simulations are shown with solid lines in Fig. 2 and are in very good agreement with experimental results.

4 Conclusion
We have performed a numerical analysis of the transport properties of a graphene flake, in which the charge deposited into a PMMA layer on top of graphene induces a cavity-shaped potential profile. Using a simplified electrostatic model and an envelope-function based transport simulator, we have been able to reproduce the behavior of the resistance seen in experiments, as a function of the voltage applied to a backgate and of the position of a negatively charged probe. An extensive exploration of the parameter range has been performed, and by comparing the results with experimental data, we have been able to understand the details of the potential profile electrostatically induced in the graphene sheet.

References:


