From quantum confinement to quantum Hall effect in graphene nanostructures

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I. INTRODUCTION

Electronic measurements in graphene and its nanostructures are being investigated by several groups\textsuperscript{1–4} and have triggered many theoretical works on the area.\textsuperscript{5–13} The applications of graphene nanostructures range from high on-off ratio field-effect transistors\textsuperscript{2,14} to spin polarized transport\textsuperscript{15} and might lead to a new type of electronics which takes the valley into account, the so-called valleytronics.\textsuperscript{16} With the recent development of device fabrication techniques it is possible to study experimentally high-quality ballistic graphene nanoconstrictions via electronic transport measurements.\textsuperscript{17} In addition, the evolution of the conductance with the magnetic field from the quantum Hall regime to conductance quantization at zero magnetic field can be used to have insights about the electronic structure and geometry of the systems considered. This technique has been shown to be very important for experimentalists in the study of quantum wires and point contacts.\textsuperscript{18–20} Inspired by the recent results in ballistic graphene nanoconstrictions,\textsuperscript{17} we present a study on graphene nanoribbons (GNRs) and graphene nanoconstrictions (GNCs) and the evolution of the conductance quantization from zero to positive magnetic field.

For a perfect ballistic armchair GNR with infinite length it is known that its conductance is quantized in steps of $\frac{2e^2}{h}$ at zero magnetic field. Due to the lack of scattering in this structure the transition between the steps in the conductance is abrupt.\textsuperscript{21} Although, when scattering is added to the picture, the conductance plateaus smear out until they are not visible anymore.\textsuperscript{7,8}

To study how the two-terminal conductance plateaus with a magnetic field for armchair graphene nanoribbons (GNRs) and graphene nanoconstrictions (GNCs). For GNRs, the conductance plateaus of $\frac{2e^2}{h}$ at zero magnetic field evolve smoothly to the quantum Hall regime, where the plateaus in conductance at even multiples of $\frac{2e^2}{h}$ disappear. It is shown that the relation between the energy and magnetic field does not follow the same behavior as in “bulk” graphene, reflecting the different electronic structure of a GNR. For the nanoconstrictions we show that the conductance plateaus do not have the same sharp behavior in zero magnetic field as in a GNR, which reflects the presence of backscattering in such structures. Our results show good agreement with recent experiments on high-quality graphene nanoconstrictions. The behavior with the magnetic field for a GNC shows some resemblance to the one for a GNR but now depends also on the length of the constriction. By analyzing the evolution of the conductance plateaus in the presence of the magnetic field we can obtain the width of the structures studied and show that this is a powerful experimental technique in the study of the electronic and structural properties of narrow structures.

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To calculate the conductance through the structures we use a nearest-neighbor tight-binding Hamiltonian and retarded Green’s-function approach as implemented in the KNIT code. The magnetic field is included within a discretized Landau gauge by adding a phase $\Phi$ in the hopping elements in a similar way as described in Ref. 23. The Aharonov-Bohm phase $\Phi$ represents the phase acquired by an electron when it goes around one hexagon, and its relation to the magnetic field, $B$, is given by $\Phi = \frac{3\sqrt{3}a_{cc}e}{2\hbar}B$, where $a_{cc} = 0.142$ nm is the carbon-carbon bond length in graphene. The contacts consist of semi-infinite graphene nanoribbons on both sides of the structures.

II. RESULTS

A. Graphene nanoribbons

We start our study by calculating the conductance, $G$, through an armchair graphene nanoribbon as a function of both the magnetic field and the Fermi energy, $E$ (Fig. 2). Here we present our results for only one value of dimer lines ($N_{DL}=101$), but we would like to emphasize that our conclusions do not change qualitatively with the width, since the behavior with the magnetic field scales with the magnetic length $l_m = \sqrt{\frac{\hbar}{eB}}$ and the energy scales with $1/W$.

In Fig. 2 two distinct behaviors of the conductance versus energy against the square root of the magnetic field can be observed: a constant position and a linear increase of the plateaus with the applied magnetic field. For an infinite graphene plane in the quantum Hall state we have

$$E_n = v_F\sqrt{2enB},$$

where $n$ is the Landau-level occupation number. So the linear relation between $E$ and $\sqrt{B}$ is an indication that the structure is in the quantum Hall regime.

For experiments performed on a GNC or GNR, it is highly relevant to know the width of the active transport region in the nanostructure. One can estimate it via the cyclotron orbit for the magnetic field where the transition to the quantum Hall state is observed. By taking the crossover point between the two behaviors with the magnetic field the width of the GNR can be extracted through the cyclotron radius:

$$l_C = \frac{E}{v_FeB},$$

where $v_F$ is the Fermi velocity and $e$ is the elementary charge. Applying this relation to the case of Fig. 2, we have $l_C = 6.015$ nm. This value is in good agreement with the width of the nanoribbon $W = 12.3$ nm, since $W = 2l_C$.

B. Graphene nanoconstrictions

In this section the results for a graphene nanoribbon connected to two wider graphene leads (see Fig. 1), i.e., a graphene nanoconstriction, are presented. To better understand this geometry, we start with the effect of the length on the conductance at zero magnetic field.

By keeping the width constant at $W = 12.3$ nm and increasing the length of the constriction from 0 [Fig. 1(b)] to 30.68 nm, two behaviors of the conductance versus energy can be distinguished in Fig. 3. For a short GNC, with a length
$L \leq W$, plateaulike features are observed in the conductance with a spacing of approximately $\frac{2e^2}{h}$. The plateaus are best defined when $L \sim W$. For $L > W$ we observe several peaks on the conductance which can be attributed to Fabry-Perot oscillations due to reflection on the graphene leads. The behavior for a short GNC shows very good agreement with the recent experiments\textsuperscript{17} where a high-quality graphene nanoconstriction was studied. Although in the experiments it was not possible to extract the length of such a nanoconstriction, we can argue that the constriction has to be short ($L \sim W$) in order to obtain well-defined plateaus in conductance observed experimentally.

Changing the width of the constriction has similar effects as changing the width of a graphene nanoribbon; i.e., the energy scale of the conductance features changes with the inverse of the width.

In Fig. 4(a), the conductance at zero magnetic field as a function of the Fermi energy is shown for a GNR in a solid black line and for a GNC with zero and finite length in red dotted and blue dashed lines, respectively. When comparing the nanoribbon with the constrictions, two key differences can be observed. First, the plateaus in conductance are sharp and well defined for a GNR but smeared out for a GNC. Second, there is a presence of a conductance gap for the nanoconstrictions, which is absent for the nanoribbon. Both differences on the conductance spectra can be explained by the enhancement of scattering in the GNC, which is absent for the GNR case. This fact explains the experimental result that even for ballistic nanoconstrictions the conductance plateaus at zero magnetic fields are not well defined.\textsuperscript{17} When the magnetic field is increased to a value in which the structures enter the quantum Hall regime the scattering is suppressed for the lower-energy channels and the conductance behaves the same for the three structures [Fig. 4(b)]. It is important to notice that, when the structures enter in the quantum Hall regime the steps in the conductance at multiples of $\frac{4e^2}{h}$ disappear and we obtain the expected steps for an infinite graphene sheet.

In Fig. 5 we have the conductance as a function of both the Fermi energy and $\sqrt{B}$ for the graphene nanoconstriction with zero length (for a finite length a similar plot is obtained). We observe quantum confinement at low magnetic fields and the quantum Hall effect at high magnetic fields, similar to the results obtained for the GNR (Fig. 2).

To study in more detail how all three structures behave at high magnetic fields, the position of the end of the plateaus $G = \frac{2e^2}{h}$ and $\frac{6e^2}{h}$ in energy with the applied magnetic field has to be analyzed. As mentioned before [Eq. (1)], the energy of the conductance plateaus should obey $E_n = \alpha_n \sqrt{B}$, where $\alpha_n = v_F \sqrt{\frac{2e}{\hbar}}$. In Fig. 6 we can see the position in energy and magnetic field for the $G = \frac{2e^2}{h}$ and $\frac{6e^2}{h}$ plateaus for a GNR and a GNC with zero length. In this plot it is clear that the plateaus in conductance do not follow the slope $\alpha$ predicted for an infinite graphene plane (dashed and dotted lines). We observe that, for the same width, the slope approaches $\alpha_n$ when the length of the GNC is reduced. For a very long graphene nanoconstriction the value of the slope approaches the value obtained for a graphene nanoribbon: $\sim 0.79 \alpha_n$. We attribute this effect to the broken valley degeneracy due to the armchair edges that modifies the energy spectrum of the Landau levels,\textsuperscript{10} since the energy dispersion for one valley is displaced to a lower energy in comparison to the other.

![Fig. 4](image_url) FIG. 4. (Color online) Conductance vs energy for (a) $B = 0$ T and (b) $\sqrt{B} = 10.5 \sqrt{T}$ for a graphene nanoribbon, in solid black lines, and a graphene nanoconstriction with zero and finite length, in dotted red and dashed blue lines, respectively.

![Fig. 5](image_url) FIG. 5. (Color online) Color plot of the conductance of a graphene nanoconstriction ($N_{DL} = 101$) with zero length as a function of the Fermi energy and $\sqrt{B}$. The lines present in the plot are isovales of the conductance. The numbers in the graph show the values of conductance in units of $G_0 = \frac{2e^2}{h}$.
Using Eq. (2), we obtain the cyclotron radius when the GNC enters the quantum Hall regime. For $L = 0$ nm we find $l_c = 7.231$ nm ($l_c > W/2$), while for $L = 5$ nm we find $l_c = 5.212$ nm ($l_c < W/2$). These values are close to the width of the constricted region ($W = 6.15$ nm) but somewhat larger when the length of the constriction is reduced.

In experiments it is common to observe several conductance plateaus at zero magnetic field, and it is possible to study their evolution as the magnetic field is varied. In addition to the use of the slope of the position of one single conductance plateau, we could also use the fact that the magnetic field to reach the quantum Hall regime depends linearly with the occupation number $n$ as $B = \frac{\hbar}{eW} n$. By using this equation to fit the position in the magnetic field at which each Landau level is created (inset of Fig. 6) in the case of the wide GNR, we obtain $W = 13.2$ nm. Despite the width of the nanostructure, by the effect known as “magnetic depopulation,”\textsuperscript{19} which consists in the deviation of the linear behavior between $n$ and $B$, one can probe the presence of one-dimensional sub-bands at zero magnetic fields even when the conductance quantization is not observed.

III. CONCLUSIONS

In summary we used a tight-binding and retarded Green’s-function approach to calculate the two-terminal conductance as a function of the Fermi energy and magnetic field for GNRs and GNCs. The conductance in the GNC showed a smoother transition between the conductance steps if we compare it to a GNR of the same width. By studying the effect of the length of the constriction on the conductance we could show that, in order to obtain the well-defined plateaus observed experimentally in a ballistic GNC, the length has to be comparable to the width. These results help us to understand the experimental results obtained and also provide a way to estimate the length of such structures, not always possible to do experimentally.

We also studied the evolution from quantum confinement to the quantum Hall state through the analysis of the conductance plateau’s position in the magnetic field. We obtained that, although the positions of the $G = \frac{2e^2}{n} \pi$ and $\frac{4e^2}{n} \pi$ plateaus follow a linear increase with $\sqrt{B}$, the slopes of the curves found for both a graphene nanoribbon and a graphene nanoconstriction were lower than the expected value for an infinite graphene plane. The value of the slope is close to the value for an infinite graphene plane for a very short constriction and deviates more for long constrictions and nanoribbons. By analyzing the position of the conductance plateaus with the magnetic field we obtained the width of the constrictions and ribbons studied through a semiclassical approach. The widths obtained are in good agreement with the real values used in our simulations, which shows that this analysis is a powerful tool for estimating dimensions of nanostructures.

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