Electronic transport of folded graphene nanoribbons

Jhon W. González
International Iberian Nanotechnology Laboratory,
Av. Mestre José Veiga, 4715-330, Braga, Portugal, and
Departamento de Física, Universidad Técnica Federico Santa María, Casilla postal 110 V, Valparaíso, Chile

Mónica Pacheco
Departamento de Física, Universidad Técnica Federico Santa María, Casilla postal 110 V, Valparaíso, Chile

Pedro Orellana
Departamento de Física, Facultad de Ciencias, Universidad Católica del Norte, Casilla postal 1280, Antofagasta, Chile

Luis Brey and Leonor Chico
Instituto de Ciencia de Materiales de Madrid, Consejo Superior de Investigaciones Científicas, Cantoblanco, 28049 Madrid, Spain

We investigate the electronic transport properties of a folded graphene nanoribbon with monolayer nanoribbon contacts. We consider two possible foldings: either the nanoribbon can be folded onto itself in the shape of a hairpin with the nanoribbon leads at a $0^\circ$ angle, or the monolayer contacts have different directions, forming a $60^\circ$ angle. The system is described by a single $\pi$-band nearest-neighbor tight-binding Hamiltonian taking into account curvature effects. We have found that for the case of a nanoribbon folded over itself the conductance oscillates from almost zero and a finite value depending on the coupling between contacts, whereas in the $60^\circ$ angle folding the conductance is only slightly perturbed, allowing for the connection of graphene nanoelectronic components in a variety of geometries.

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I. INTRODUCTION

Graphene is an one-atom-thick covalently-bonded carbon layer ordered in a honeycomb lattice. It has been recently isolated and shown to be stable under room conditions, giving rise to the exploration of its fascinating properties. As it is an ambipolar material, the charge carrier type can be changed by applying a gate voltage; furthermore, the high mobility of charge carriers due to the absence of backscattering. These characteristics point at graphene as an interesting alternative for novel nanoelectronic devices. However, as graphene is a zero-gap material, it cannot be employed for the fabrication of diodes and most electronic components, for which an electronic gap is essential. Thus, there has been substantial interest in controlling the electronic properties of graphene by quantum size effects. For example, cutting graphene into quasi-one-dimensional nanoribbons produces electronic gaps. Another route to produce a gap is to stack two graphene layers. Bilayer graphene$^{11,12}$ holds huge potential because it is a gate-tuneable semiconductor$^{13,14}$ as observed in electronic transport$^{15,16}$ and in photoemission experiments$^{17}$. Furthermore, folds and bends on narrow carbon nanoribbons have also been reported$^{18}$. From the theoretical viewpoint, the electronic structure of folded graphene has been studied$^{19}$. The transport properties of folded graphene nanoribbons along the fold direction have also been reported without considering curvature effects$^{20,21}$; besides, the transport in a uniform magnetic field has also been explored$^{22}$, but the emphasis was in the effective change of direction the magnetic flux when moving across the fold, and no curvature effects nor interlayer coupling were considered.

We consider the folded ribbon to be composed of a curved portion, also called fractional nanotube$^{23,24}$ and two armchair graphene ribbons with a finite overlap re-
FIG. 1: Schematic view of the two configurations considered. (a) Nanoribbon folded at 0°. The length of the bilayer part is \(L_b\). To this bilayer portion, two monolayer nanoribbons are connected, indicated by \(m\). (b) Geometry of the 60° folded ribbon. The bilayer region is a triangular portion marked with \(b\); the monolayer contacts are labeled by \(m\). Note that the distance \(t_b\) between the upper and lower ribbon is constant in the planar part.

II. THEORETICAL DESCRIPTION OF THE SYSTEM

A. Tight-binding Hamiltonian

The low-energy transport properties of planar graphene are well described within a single \(\pi\)-band tight-binding approximation with nearest-neighbor in-plane hopping given by the parameter \(\gamma_0 \approx 3\) eV. This model only considers the \(\pi\) and \(\pi^*\) bands due to the hopping between \(p_z\) orbitals perpendicular to the graphene plane. In the fractional nanotube region, we must consider the effect of curvature. As its main consequence is the misalignment of the \(p_z\) orbitals, we model it by assuming that the hopping integral between neighbor atoms is changed with respect to that of planar graphene. The curvature-modified hopping \(\tilde{\gamma}_0\) is proportional to the cosine of the misalignment angle \(\phi\) between orbitals, 

\[
\tilde{\gamma}_0 = \gamma_0 \cos \phi,
\]

with \(\phi\) defined in Fig. 2(a).

The region where the two ribbons overlap is just a finite-size fragment of bilayer graphene with AA stacking. In the case of folding at 0°, the bilayer region is a rectangular flake of length \(L_b\). For nanoribbons folded at 60°, the bilayer flake has a triangular shape, as depicted in Fig. 1(b), with size depending on the ribbon width. The interlayer coupling is modeled with a single hopping \(\gamma_1\) connecting atoms directly on top of each other, which we take as \(\gamma_1 = 0.1\gamma_0\), in agreement with experimental results.\(^{11,21}\)

In the bilayer with AA stacking all the atoms of layer 1 are on top of the equivalent atoms of layer 2. We assume that all atoms bottom layer are connected to those on the upper layer located exactly on top of them; thus, the Hamiltonian takes the form

\[
H^{AA} = -\sum_{<i,j>,m} (a_{m,i}^+ b_{m,j} + h.c.) - \gamma_1 \sum_i (a_{1,i}^+ a_{2,i} + b_{1,i}^+ b_{2,i} + h.c.).
\] (1)

where \(a_{m,i}(b_{m,i})\) annihilates an electron on sublattice \(A(B)\), in plane \(m = 1, 2\), at lattice site \(i\). The subscript \(<i,j>\) represents a pair of in-plane nearest neighbors. The second term in Eq. (1) represents the interlayer hopping.
B. Landauer-Büttiker formalism

We calculate the electronic and transport properties using the surface Green function matching method\textsuperscript{22,23}. Thus, the system is partitioned in three blocks: two semi-infinite leads, which we assume to be semi-infinite aGNRs, and the conductor, consisting of the bilayer and the folded region. The Hamiltonian of the system can be partitioned as

\[ H = H_C + H_R + H_L + V_{LC} + V_{RC}, \]

where \( H_C, H_R, \) and \( H_L \) are the Hamiltonians of the central portion, left and right leads respectively, and \( V_{LC}, V_{RC} \) are the coupling matrix elements from the left \( L \) and right \( R \) lead to the central region \( C \). The Green function of the conductor is

\[ G_C(E) = (E - H_C - \Sigma_L - \Sigma_R)^{-1}, \]

where \( \Sigma_\ell = V_C g_\ell V_C^\dagger \) is the selfenergy due to lead \( \ell = L, R \), and \( g_\ell = (E - H_\ell)^{-1} \) is the Green function of the semi-infinite lead\textsuperscript{23}.

The conductance can be calculated within the Landauer formalism in terms of the Green function of the system\textsuperscript{25,26}.

\[ G = \frac{2e^2}{h} T(E) = \frac{2e^2}{h} \text{Tr} \left[ \Gamma_L G_C \Gamma_R G_C^\dagger \right], \]

where \( T(E) \) is the transmission function across the conductor, and \( \Gamma_\ell = i[\Sigma_\ell - \Sigma_\ell^\dagger] \) is the coupling between the conductor and the \( \ell = L, R \) lead.

III. RESULTS

A. Nanoribbons folded at 0°

We first focus on an armchair graphene nanoribbon folded onto itself in the shape of a hairpin, i.e., in a configuration where the relative angle between the bottom and top leads is 0° (Fig.\textsuperscript{IIa}). Here we need to consider two effects: the layer-layer coupling which depends on the length of the overlapping region, and the effects of the curved portion, modeled as a fractional nanotube. We assume our leads are noninteracting monolayer graphene nanoribbons, so that the bilayer region with interlayer coupling has a finite size \( L_b \), given in terms of the armchair unit cell size length. The width of the nanoribbon is given by the number of dimers across its width, \( N \).

For an armchair nanoribbon folded at 0°, the curved edge has to be a fractional armchair nanotube (fzCNT). In this work we model the curved edge as a section of a (4,4) armchair carbon nanotube. In Figure\textsuperscript{II(b)} we show the conductance of the aGNR of width \( N = 11 \) folded at 0° as a function of Fermi energy for several bilayer lengths \( L_b \). Notice the periodic behavior in the conductance as a function of the energy, due to the multiple interferences produced in the bilayer region. These periods change with the system size. Besides, there is another periodicity related to the bilayer portion \( L_b \), roughly equal to 8 unit cells. These periodicities in the electronic conductance are also observed with equal frequencies in wider aGNR ribbons folded at 0°, such as the N=17 case (not shown here because in the depicted energy range their conductances are equal, given that they only have one conductance channel at that energy interval). The oscillations are reminiscent of those found in the transmission through bilayer flakes\textsuperscript{2}, where the conductance was demonstrated to depend on both the energy and the size of the scattering region.

B. Nanoribbons folded at 60°

For the 60° configuration, the folded edge for an armchair nanoribbon has to be a fractional zigzag nanotube (fzCNT) in order to maintain the AA stacking in the bilayer region. The radius of the fzCNT depends on nanoribbon width, and close to 0.35 nm, to be consistent with previous ab-initio calculations\textsuperscript{19}.

In figure\textsuperscript{II(a)}, we show the conductance as a function of Fermi energy for aGNR \( N = 11 \) at 60° with a fzCNT (8,0). The bilayer region for this case consists of a triangle, as shown in Fig\textsuperscript{II(b)}. The most relevant change with respect to to hairpin geometry is that the electron-hole symmetry is broken. This is due to the mixing of the two
FIG. 4: (color online) (a) Conductance as a function of the Fermi energy for an aGNR of width $N = 11$ at $60^\circ$ with a fractional zigzag carbon nanotube (8,0). (b) Conductance as a function of the Fermi energy for an aGNR of width $N = 17$ at $60^\circ$ with a fractional zigzag carbon nanotube (9,0). For reference we included a dotted line for the respective pristine monolayer aGNRs, namely, the $N = 11$ and the $N = 17$ cases.

In figure 4(b) we show the conductance as a function of Fermi energy for an aGNR of width $N = 17$ at $60^\circ$ with a fzCNT (9,0). Due to the size of the overlapping ribbons, we need to consider here a slightly larger nanotube than in the previous case. The chosen fzCNT is consistent with ab-initio predictions and permits the obtention of the AA stacking in the bilayer region. We also observe in this case that electron-hole symmetry is broken, but the decrease in the electronic conductance around zero is very small, as in the $N=11$ aGNR folded at $60^\circ$ ribbons.

Obviously, the folded nanoribbons always should show a conductance smaller than the pristine unfolded case, as can be seen in Figs. 4 (a) and (b). This is due to the interferences occurring in the scattering folded region, both at the bilayer stacked portions and in the curved nanotube, where there is a different effective hopping because of curvature effects. But due to the small size of the scattering regions in the nanoribbons folded at $60^\circ$, the change in the conductance around zero energy is not dramatic, thus allowing for the connection of nanoribbons at different heights without a substantial decrease in their transport properties.

IV. CONCLUSIONS

We have studied the transport properties in folded graphene nanoribbons. We have found that the connections with folded ribbons do not show the large conductance gaps present in other types on nanoribbon junctions. We have also explained the lack of electron-hole symmetry present in folded graphene edges\textsuperscript{15}, which can be understood in terms of the introduction of odd-membered carbon rings in the graphene lattice. First-principles calculations show that the curved edge may have a larger radius\textsuperscript{27}, so our approach overestimates the reduction of the conductance due to the curvature-induced change of the hopping integrals, pointing at an optimal conductance of folded ribbons as carbon connections.

Acknowledgments

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