Electronic states and quantum transport in graphene ribbons

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Graphene is a single atom thick sheet of carbon. For almost half century after the pioneering paper of Wallace, strictly two dimensional graphite was but a beautiful exercise for students of theoretical solid state physics and chemistry. Only recently high quality and stable under ambient conditions two dimensional carbon sheets have been isolated, and the potential of graphene-based electronics on the micro- and nano-metric scale has further magnified the interest toward this material. Graphene ribbons are infinitely extended in one direction and have two typical terminations in the orthogonal one: the zigzag and the armchair terminations.
By means of the tight binding model for the description of the electronic states and the nonequilibrium Keldysh Greenís function for quantum transport, we studied the electronic structure and current profiles of graphene ribbons. We show that charge manipulation in the engineering of graphene is conceptually possible by external gates and magnetic fields.

Graphene, neutral or controlled by external voltages, can be considered as a reservoir of massless relativistic particles. The peculiar relativistic-like dynamics of the charges involved in magnetotransport experiments have attracted great interest and envisaged novel devices for nanoelectronics [1,2] and valley-valve filters [3].
Carrier density in graphene can be varied from electrons to holes using external local gates (see Fig.1).

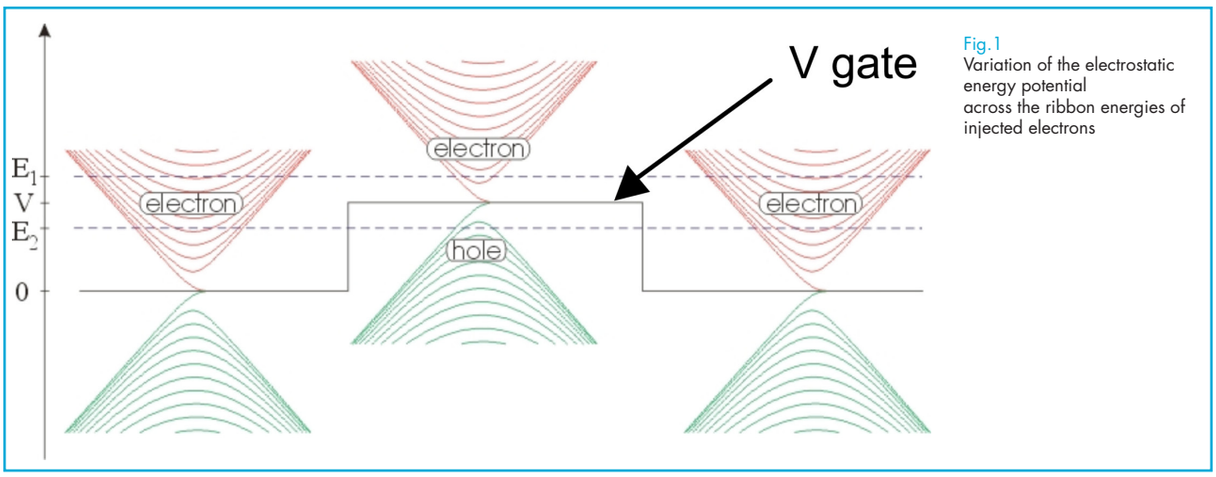

Fig.1
Variation of the electrostatic energy potential across the ribbon energies of injected electrons

We have simulated stationary currents distribution [4,5] in graphene ribbons in the presence of magnetic fields and top gate potentials, by means of the nonequilibrium Keldysh-Green's function formalism within a tight-binding model. The exploited formalism allows imaging of local currents and evaluation of quantum shot noise. The Keldysh method, joint with the decimation-renormalization technique, emerges as a very suitable tool for microscopic treatment of charge transport in the presence of superimposed potentials. This method, widely applied in the study of charge transport in conventional two-dimensional electron gases in square lattices, has been adapted to the honeycomb topology [4]. In the case of superimposed gates, it provides a real space view of the currents and suggest the way to realize their manipulation.

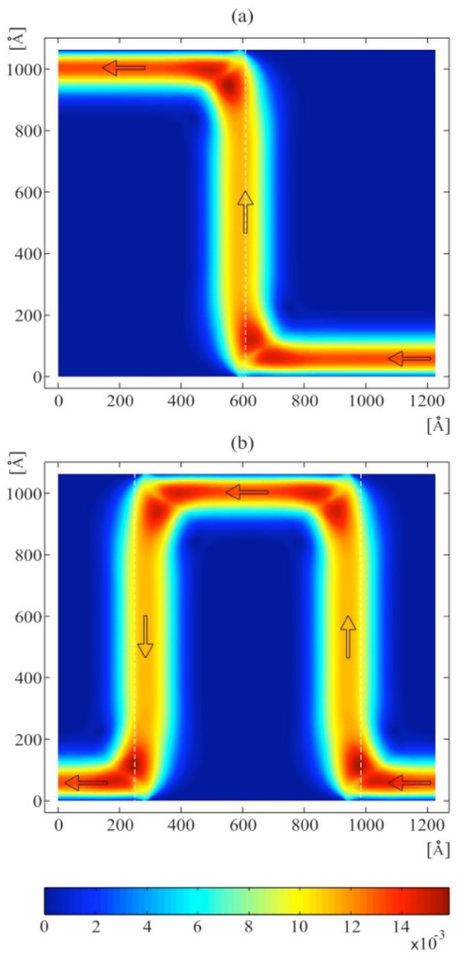

Fig.2
Current distribution in a p-n (a), and in a n-p-n (b) junction realized by a gated graphene ribbon in the presence of a magnetic field

We have shown that in *n-p-n* devices, realized when the height of the gate potential barrier is larger than the energy of the injected carriers, electron particles turn into holes inside the barrier and turn back to electrons outside it. Imaging of current profiles(a) (see Fig.2) gives a vivid picture of the easy Klein tunneling through barriers by virtue of the electron-like or hole-like behavior of the relativistic particles in the *n*-doped and *p*-doped regions.

The current maps are of particular interest in the presence of magnetic fields since the spatial distribution of currents is sensitive to the nature of the carriers. In strong magnetic fields, electrons and holes flow along opposite edges of the sample and this shows that current manipulation is in principle possible by means of top gates.

Transport properties of graphene nanoribbons depend dramatically on their zigzag or armchair termination and on the presence of long range or short range disorder. Recently, it has been shown that a *p-n* junction in a clean zigzag nanoribbon blocks the current completely if the number of carbon chains in the ribbon is even [3]. In the case of an odd number of chains, on the contrary, the system is almost transparent. We have evidenced this phenomenon by electronic transport simulations and have given an interpretation based on symmetry arguments [6].

The bipolar junction is obtained by means of a superimposed potential step with height V on the left region (Fig.3a), where the band structure turns out to be shifted by V (Fig.3b). We consider a potential that only varies along the longitudinal direction. If we inject the particles from the right side of the ribbon (red arrows) at an energy $0 < E < V$, the charges enter the system as electrons and are transmitted to the left as holes. As indicated in Fig.3b, in this range of energy the transport is realized by scattering from the K valley to the K' valley. In Fig.3c is reported the conductance G of a ribbon made up of N= 100 carbon chains for $V = \Delta$, where Δ is the separation between the energy levels at K. In the region $0 < E < V$ we have $G = 0$. For N= 101, in the same region we have $G = 2e^2/h$ [6].

To interpret this effect, we consider the spatial reflection symmetry of the zigzag nanoribbon with respect to the central plane along the longitudinal direction if N is even, or the reflection operation followed by a fractional translation for odd N. The energy bands can be classified as even or odd with respect to these spatial operations. To have intervalley scattering in the energy region where only one mode is active in both the *p* and *n* regions, the step potential must break the symmetry of the ribbon. It can be shown that the symmetry is respected when N is even,

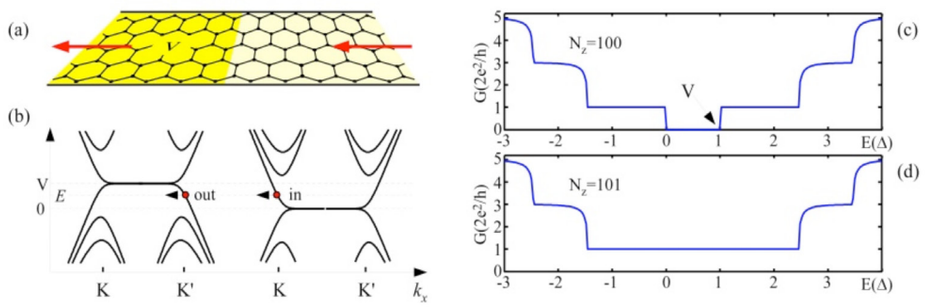

Fig. 3
(a) Scheme of the ribbon with superimposed step potential V. (b) Scheme of the energy bands in the two regions and channels involved into transmission. (c) Differential conductance for N = 100 carbon chains. (d) Differential conductance for N = 101 carbon chains.

and no current transmission is allowed, while the symmetry is broken when N is odd. These general considerations are supported by direct calculations of the coupling between the crystalline wave functions of the ribbon induced by the superimposed step potential.

We have also investigated the transport properties of gated conjugated polymers of the polyacene series [7] as examples of ultranarrow zigzag graphene ribbons. Our simulations demonstrate that the polymeric system is insulating or conducting according to the Fermi energy of the injected electrons, of the even or odd number of chains, and of the shape of the gate potential. In summary, we notice explicitly that for appropriate energy intervals to the right of the reference energy E = 0, all even ribbons are perfectly insulating. This behavior, appealing for electronic valve applications, was first observed for wide graphene ribbons. It occurs regardless of the two-valley band structure of graphene, and also holds for ultranarrow graphene ribbons. We have in fact shown that the origin of the effect are symmetry and topology.

References

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