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Graphene Nanoribbons with End- and Side-Contacted Electrodes

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This contribution reports on theoretical studies of electronic transport through graphene nanoribbons in the two-terminal geometry. The method combines the Landauer-type formalism with Green's function technique within the framework of the standard tight-binding model. The aim of this study is to gain some insight on how fundamental electric current characteristics (conductance and shot noise) depend on interface conditions imposed by graphene nanoribbon/metal-electrode contact details. Calculations have been carried out for both end- and side-contact geometries, and metallic (zigzag-edge) as well as semiconducting (armchair-edge) graphene nanoribbons. It turns out that results for side-contacted systems depend on the ratio between the free-standing graphene nanoribbon length to that covered by the electrode. For sufficiently long nanoribbons the results start converging when this ratio exceeds 0.5. In the case of ferromagnetic contacts, the giant magnetoresistance coefficient is also discussed.

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1. Introduction

Graphene, a single-atom thick layer of graphite, has been under intensive studies for 7 years, i.e since it was first shown experimentally to form a stable two--dimensional structure [1]. One of the fundamental problems related with potential applications of graphene nanoribbons in nanoelectronics and spintronics concerns the impact of graphene nanoribbons (GNR)/electrode interfaces on electronic transport and magnetic properties. This problem has not yet been unambiguously solved, despite much attention devoted to it [2–7]. The present studies aim at gaining some additional insight into this issue.

2. Method

The most important facts concerning the present method are as follows: (i) Two terminal systems are studied with metallic external electrodes either end-contacted or side-contacted to graphene nanoribbons. (ii) The electrodes are infinite (or semi-infinite) 3-dimensional slabs. (iii) Recursive Green's function method is combined with the Landauer formalism:

$$G = 1/(E - H - \Sigma_{\rm L} - \Sigma_{\rm R}),$$
$$T = \Gamma_{\rm L} G \Gamma_{\rm R} G^{\dagger},$$
$$\sigma = \frac{e^2}{h}\,{\rm Tr}(T),$$
$$\Gamma_{\rm L,R} = {\rm i}\left(\Sigma_{\rm L,R} - \Sigma_{\rm L,R}^{\dagger}\right),$$
$$F = 1 - {\rm Tr}(T^2)/{\rm Tr}(T),$$
$${\rm GMR} = 100(1 - \sigma_{\uparrow,\downarrow}/\sigma_{\uparrow,\uparrow}).$$

Above, G is Green's function, H is a tight-binding Hamiltonian matrix, $\Sigma_{\rm L,R}$ are self-energies for the left (L) and right (R) electrodes, T is a transmission matrix whereas σ and F stand for the conductance and the shot noise Fano factor. The Hamiltonian is a one--orbital block tri-diagonal matrix whose sub-matrices contain nearest neighbor hopping integrals, allowed to take 3 values (t = 2.7 eV, $t_{\rm M} = t/2$ and $t_{\rm C} = \sqrt{t t_{\rm M}}$) inside the GNR, inside the electrode and at the GNR/electrode interface, respectively. If the electrodes are ferromagnetic, a giant magnetoresistance (GMR) coefficient is also computed in terms of the respective conductances for the parallel magnetization alignment of the electrodes ($\uparrow\uparrow$) and the antiparallel one ($\uparrow\downarrow$). In that case on-site parameters in the model electrodes have been chosen such that their spin polarization equals 50%. The transport regime of interest here is the ballistic one [8–10], with a strong coupling between the nanostructure and the leads (the opposite limit, Coulomb blockade, was considered in [11]). For more detailed description of the present formalism on self-energies and the recursive Green function method see [7, 12].

3. Modelling and results

The systems under consideration are schematically shown in Fig. 1. They consist of metallic electrodes (big spheres) coupled to the GNR (small spheres). Two first setups correspond to end- and side-contacted zigzag GNRs, whereas the others are their armchair counterparts. The presented systems differ fundamentally from each other, since the former is always metallic and the latter — semiconducting (for the widths discussed here).

In case of the zigzag GNR, increasing the unsupported length results in a saturation of the conductance (G) at e^2/h per spin — meaning that the interfaces become more and more transparent. For the armchair semiconducting GNR, in turn, beyond the energy gap the conductance for the side-contacted systems is quantitatively close to that of the end-contacted one ($L_0 = 0$) for ultra short lengths only, otherwise G reveals much more pronounced dips.

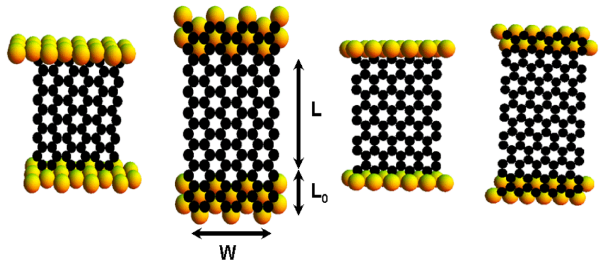

Fig. 1. Schematics of the end- and side-contacted zigzag setups as well as the armchair ones (left to right). The labels W, L, L_0 stand for the relevant dimensions of the GNRs: the width along the horizontal edge, the unsupported length along the vertical edge, and the electrode-supported length, respectively.

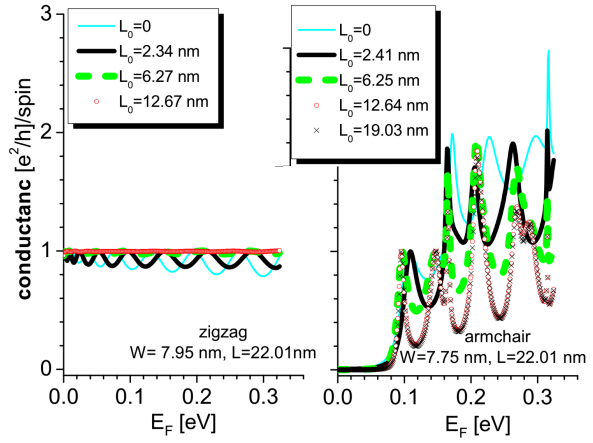

Fig. 2. Conductance of zigzag (left) and armchair (right) GNRs for setups of comparable sizes (width = W, unsupported length = L, and supported length = L_0).

Remarkably, both in zigzag- and armchair systems the saturation takes place roughly at $L_0/L \approx 0.5$, whereas in order to approach the end-contacted limit, the electrode supported length must be short enough so that $L_0/L \approx 0.1$. As concerns the Fano factor, F (see Fig. 3), the results converge analogously as for G. However in the zigzag case F goes to the noiseless limit, whereas for the semiconducting armchair GNRs there are pronounced oscillations, ranging from 0 up to 0.8 with E_F (or gate voltage). The convergence with increasing L_0 is easily seen in the left parts of Figs. 2 and 3 (flat curves).

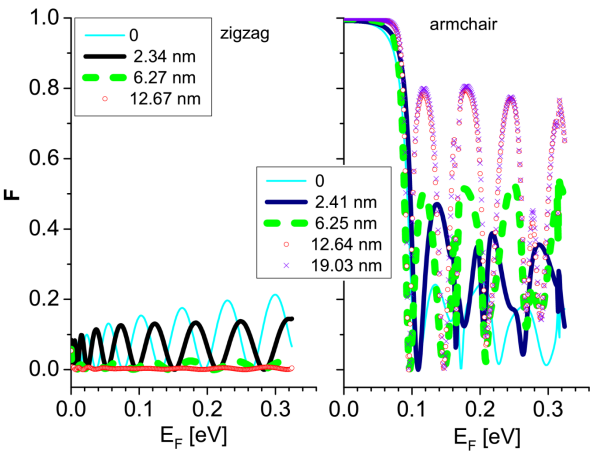

Fig. 3. As in Fig. 2 but for the noise Fano factor.

As concerns the right parts, the convergence is also evident. Let us note that crosses and circles overlap with one another.

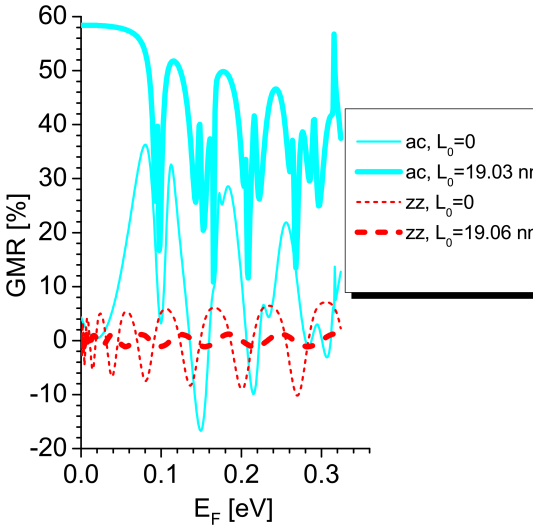

Fig. 4. GMR for armchair (ac) and zigzag (zz) GNRs for end- and side-contacted setups.

Figure 4 presents GMR coefficients of zigzag and armchair setups for $L_0 = 0$ (end-contacted), and $L_0 \approx 19$ nm (close to the saturation coverage). As can be readily seen, the GMR coefficients in the zz-GNRs are small and get reduced while increasing the coverage length. In contrast, for ac-GNRs with a sufficiently long electrode-supported part, GMR can assume quite large values.

4. Conclusions

Summarizing, it has been shown that in the ballistic transport regime electronic transport characteristics depend in general on whether the setups are of end- or side-contacted type. However, since the results converge

rather quickly with the length of the metal-electrode supported part of the GNR, experimentally side-contacted and embedded-end-contacts results would be hard to tell from one another. The GMR coefficient of zigzag GNRs turns out to be small, whereas that for armchair GNRs can reach several tens percent.

Acknowledgments

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