Transport properties of graphene nanoribbon heterostructures

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Abstract

We study the electronic and transport properties of heterostructures formed by armchair graphene nanoribbons with intersections of finite length. We describe the system by a tight-binding model and calculate the density of states and the conductance within the Green’s function formalism based on real-space renormalization techniques. We show the apparition of interface states and bound states in the continuum which present a strong dependence of the heterostructure geometry. We investigate the effects on the conductance of an external perturbation applied on the edges atoms of the intersection region.

Key words: Graphene nanoribbons, Electronic properties, Transport properties, Heterostructures

PACS: 73.22.-f, 61.46.+w, 73.40.-c
1 Introduction

The fabrication under controlled experimental conditions of graphene nanoribbons (GNRs) has attracted a lot of scientific interest in the last decade. GNRs are single atomic layers which can be understood as an infinite unrolled carbon nanotube. The special electronic behavior of GNRs defined by their quasi one-dimensional electronic confinement and the shape of the ribbons ends (two cases of maximum symmetries can be obtained: zigzag and armchair ends), suggest remarkable applications in graphene-based devices. Moreover, due to the flat structure GNRs seem to be easier to manipulate than carbon nanotubes. The transport properties of these structures have been studied with special interest by several scientific groups. Peres et al find that for clean systems, the quantization condition for the electronic conductance is different for zigzag and armchair GNRs. Shi et al show that applying a gate voltage to the ribbons it is possible to obtain an electronic switch very useful to study the Klein paradox.

In this work we present a theoretical description of the electronic and transport properties of graphene heterostructures formed by armchair GNRs of different widths. The systems are composed by M unit cells of a semiconducting $N_C$ armchair GNR surrounded by two semi-infinite $N_L$ metallic ribbons [with the condition $N_C = N_L + 4$]. These kinds of systems allow us to consider two possible configurations: a Cross-bar and a T-shaped heterostructure, which are schematically shown in Fig.1. We investigate the effects of a weak external perturbation applied on the edges atoms of these two heterostructures. The external perturbation slightly modifies the on-site energies of these atoms, allowing the mixture of continuous and localized states of
the system. We found the presence of two kind of localized states: interface states and bound states in the continuum. The former states reside in the interface of the two perpendicular nanoribbons. The latter states are bound states due to the quantum interference of the electron wavefunction inside of the nanoribbons intersection \((5, 7)\). The external potential allows the contribution of these localized states to the transmission of the electrons through the central conductor which can be observed in the conductance of these systems.

![Atomic configuration of the armchair heterostructures](image)

Fig. 1. Atomic configuration of the armchair heterostructures: (a) Cross-bar and (b) T-shaped configuration. The black atoms at the edges of the central region represent the effect of the applied external perturbation \(\Delta V\). The black rectangle define the unit cell of the central part.

2 Model

The systems are described in a real-space picture which allows to incorporate the potential fluctuations at the microscopic scale. We adopt a single \(\pi\)-band tight-binding Hamiltonian taking into account only nearest-neighbor hopping
interaction (with $\gamma \approx 2.75\text{eV}$). The density of states (DOS) and the conductance of the systems are obtained in the Green’s function formalism based on real-space renormalization techniques(8). The conductance is calculated using the surface Green’s functions matching formalism(9). Within this picture the full system is partitioned into three parts: the central structure (the GNR intersection region) and two leads (two semi-infinite metallic GNRs). In the linear response approach, the conductance can be calculated using the Landauer formula given by: $\Gamma(E_F) = \frac{2e^2}{h}T(E_F)$, where $T(E_F)$ is the transmission function of an electron crossing through a central conductor (for more details see ref.(9; 10; 8)). The strength of the external perturbation is written in term of the potential difference between the edges atoms of the central structure, $\Delta V$. In what follows all the energies are written in terms of the hopping parameter $\gamma$ and the Fermi energy level is taken as the zero of the energies.

3 Results and Discussion

Results of the DOS for the heterostructures formed by $M=3$ unit cells of $N_C=9$ and leads with $N_L=5$, for different external potential strengths $\Delta V$, are shown in Fig. 2. In the lower panel we show the behavior of the DOS of the two considered structures as a function of the energy. We include in the plot the DOS of a pristine armchair GNRs $N=5$ (solid black online) for comparison. For the cross-bar heterostructure (dash blue online), two kind of states can be distinguished: interface states and bound states in the continuum (resonant states). The interface states come from the junction region between the leads and the central ribbon structure. These states are pinned at the Van Hove singularities of the pristine $N=5$ armchair GNR. On the other
hand, the bound states in the continuum (two symmetric states with respect to the Fermi level at ±0.368γ) arise from the interference of the electron wave function inside the central ribbon. The occurrence of these states is only an effect of the space symmetry of the heterostructure configuration. This can be corroborated comparing the behavior of the DOS of the T-shaped structure (dot red online) with the cross-bar structure. It is possible to observe the interface states at the same energies as that for the cross-bar heterostructure but the bound states disappear due to the breaking of the spatial symmetry of the system. We analyze the effect of the external potential strength ∆V on the bound states and interface states of the heterostructures. In the central panel we show the behavior of one bound state (0.368γ) and one interface state (1.0γ) of the cross-bar heterostructure for different potential strengths ∆V. It is possible to observe that the bound state is not degenerated and the effect of the external potential is only a slight displacement of the energy level proportional to ∆V. On the other hand, besides of the energy shift, the interface state shows a break of its degeneracy at ∆V=0.06γ. This fact affects the conductance of the system as we see later. In the upper panel we show the behavior of the interface state pinned at 1.0γ for the T-shaped heterostructure. As expected due to its nature, the same behavior of the cross-bar heterostructure is obtained, a break of the degeneracy and an energy shift proportional to ∆V can be observed.

In what follow we consider the behavior of the conductance of the heterostructures described before as a function of the external perturbation potential. Results of the conductance for the cross-bar heterostructures \( N_L = 5 \) and \( 3 \times N_C = 9 \), for different external potential strengths ∆V are shown in Fig. 3. For all considered values of ∆V the system shows a semiconductor behavior.
Fig. 2. (a) DOS as a function of the energy of the cross-bar and the T-shaped heterostructures in comparison with the DOS of a pristine armchair GNR N=5, (b) DOS of the cross-bar heterostructure for two special energy values for different external potential strength and (c) DOS of the T-shaped heterostructure for a special energy values for different external potential strength $\Delta V$.

A Fano antiresonance pinned at $0.47\gamma$ and a thin Fano resonance pinned at $0.65\gamma$, which arise from the electron interference inside of the central structure, are almost invariant when the external potential is applied over the central structure. For $\Delta V > 0$ very thin peaks and dips can be observed in the conductance curves at defined energy levels. For instance, at energy equal to $1.0\gamma$ the conductance shows an evolution between peaks and dips depending on the strength of $\Delta V$. This behavior is due to the shift and break of degeneracy of the interface states at that energy. The intensity of the dips becomes a quan-
tum of conductance for $\Delta V \geq 0.06 \gamma$. For energy equal to $0.65 \gamma$ a thin peak in the conductance is observed, which evolves with the potential strength. These peaks are produced by a bound state that becomes a resonant one for finite $\Delta V$ values and it starts to contribute to the transmission of the system when the external potential is applied.

![Conductance Graph](image)

Fig. 3. Evolution of the conductance of the cross-bar heterostructure for different values of the external potential strength.

Results of the conductance for the T-shaped heterostructures for different potential strengths $\Delta V$ are shown in Fig. 4. Similar to the cross-bar heterostructures, the system has a semiconductor behavior for all considered $\Delta V$ values. In comparison with the cross-bar heterostructure, the conductance shows more antiresonances (i.e. point of zero conductance). These antiresonances arise from the Fano effect due to the destructive interference of the electron when it follows different pathways. It is possible to observe at energy equal to $1.0 \gamma$, a thin peak that evolves with the external perturbation, which grows in inten-
sity and becomes narrower due to the break of the degeneracy of the interface state pinned at this energy level when the potential strength increase.

Fig. 4. Evolution of the conductance of the T-shaped heterostructures for different values of the external potential strength

4 Summary

We have calculated the DOS and conductance of heterostructures formed by armchair GNRs. We analyzed their electronic properties when a weak external potential is applied on the edges atoms of the central ribbon structure. We found the presence of interface states and bound states in the continuum. This corresponds to the formation of collective states by the coupling of individual states and the interference among the intersection region.
5 Acknowledgments

This work was supported by CONICYT/Programa Bicentenario de Ciencia y Tecnología (CENAVA, grant ACT27).

References

[1] T. Ohta et al, Science 313 (2006) 951 ; S. Stancovich et al, Nature 442 (2006) 282.
[2] K. Nakada et al, Phys. Rev B 54 (1996) 17954 ; K. Wakabayashi and H. Hiroshima, Phys. Rev B 64 (2001) 125428.
[3] Q. W. Shi et al, cond-mat/0611604 v1, (2006); A. Rycerz et al, cond-mat/0608053 v1, (2006).
[4] N. Peres, A. Castro and F. Guinea Phys. Rev B 73 (2006) 195411.
[5] J. U. Nöckel, Phys. Rev. B 46 (1992) 15348.
[6] Zhen-Li Ji and Karl-Frederik Berggren, Phys. Rev. B 45 (1992) 6652.
[7] M. L. Ladrón de Guevara and P. Orellana, Phys. Rev. A 73 (2006) 205303.
[8] C. G. Rocha, A. Latgé, and L. Chico, Phys. Rev. B 72 (2005) 085419 ; L. Rosales, C. G. Rocha, A. Latgé, Z. Barticevic and M. Pacheco, Phys. Rev. B75 (2007) 165401.
[9] M. Nardelli, Phys. Rev B 60 (1999) 7828.
[10] S. Datta, Electronic Transport in Mesoscopic Systems, Cambridge University Press, 1995.