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Reprint of : Finite-size effects on the minimal conductivity in graphene with Rashba spin–orbit coupling

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HIGHLIGHTS

- Using Landauer–Büttiker formalism, the minimal conductivity of monolayer graphene with Rashba spin–orbit couplings was obtained in continuum and tight binding models.
- Finite and infinite samples are considered.
- For finite samples depending on its orientation with respect to the electrodes, the conductivity can be suppressed compared to that obtained for infinite samples.
- This effect can be explained by a simple analysis of the boundary conditions.
- Owing to the spin–orbit interactions an oscillation of the conductivity is observed and explained as interference of states corresponding to different energy pockets of the low energy Fermi surface.

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ABSTRACT

We study theoretically the minimal conductivity of monolayer graphene in the presence of Rashba spin–orbit coupling. The Rashba spin–orbit interaction causes the low-energy bands to undergo trigonal-warping deformation and for energies smaller than the Lifshitz energy, the Fermi circle breaks up into parts, forming four separate Dirac cones. We calculate the minimal conductivity for an ideal strip of length L and width W within the Landauer–Büttiker formalism in a continuum and in a tight binding model. We show that the minimal conductivity depends on the relative orientation of the sample and the probing electrodes due to the interference of states related to different Dirac cones. We also explore the effects of finite system size and find that the minimal conductivity can be lowered compared to that of an infinitely wide sample.

1. Introduction

More than half a century has passed since Landauer derived a formula for the conductance of two terminal coherent devices [1]. Then 25 years ago *Markus Büttiker* realized that the two terminal Landauer formula can be extended to multi-terminal devices [2]. Now, in the literature this approach is commonly called Landauer–Büttiker formalism. Over the years it becomes the standard tool for investigating various quantum systems in nanophysics (for a review see Refs. [3–6]). This approach has become an integral part of theoretical investigations of modern solid states systems such as graphene [7]. In the last decade different types of graphene nanostructures proved to be one of the most technologically promising and theoretically intriguing solid state systems. The dynamics of low energy excitations in graphene is governed by an effective Hamiltonian corresponding to massless two dimensional Dirac fermions. Hence many physical quantities such as the conductivity, the quantized Hall response and optical properties are markedly different from those of conventional two dimensional electron systems [8]. In bilayer graphene, the interlayer hopping results in a trigonally warped Fermi surface which breaks up into four separate Dirac cone at low energies. The signatures of this novel electronic structure have been studied first experimentally by Novoselov et al. [9] and theoretically by McCann and Fal'ko [10].

Graphene samples, despite the vanishing density of states,

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show a finite conductivity at the charge neutrality point (at zero Fermi energy). This feature of massless Dirac fermions, referred to as minimal conductivity, was intensively studied with the Landauer–Büttiker formalism [11–13]. An alternative approach based on the Kubo formula has also been applied to study this phenomenon in both monolayer and bilayer graphene [14,15]. It was shown that in monolayer graphene for wide and short junction the value of the minimal conductivity is $\sigma_0 = (4/\pi)e^2/h$ [11,13]. For bilayer graphene neglecting trigonal warping the conductivity is $\sigma = 2\sigma_0$, while including splitting of the Dirac cone due to trigonal warping gives extra contributions to the conductivity, increasing it to $\sigma = 6\sigma_0$ [15]. Later, for finite size of bilayer graphene it was shown by Moghaddam and Zareyan [16] that the trigonal warping results in an anisotropic behavior of the minimal conductivity.

Rashba spin–orbit (RSO) interaction arises once the mirror symmetry of the bulk graphene sample is broken by the substrate or an applied electric field perpendicular to the graphene sheet. The strength λ of the RSO coupling is proportional to this electric field. Photoemission experiments on graphene/Au/Ni(111) heterostructure revealed $\lambda \sim 4$ meV [17]. Recently, a strong Rashba effect with spin–orbit splitting of 70 meV has also been observed for graphene on Fe(110) [18]. Moreover, a non-uniform spin–orbit coupling of $\lambda \approx 100$ meV induced by Pb monolayer in graphene has been estimated experimentally by Calleja et al. [19].

Enhanced RSO interaction has a major impact on the transport properties of graphene derived samples. Recently the transfer matrix method has been employed to study spin dependent transport properties of monolayer graphene in the presence of inhomogeneous RSO coupling [20,21]. An important consequence of the RSO interaction is that the low-energy behavior of electrons in monolayer graphene with RSO coupling is related to that of bilayer graphene with trigonal warping but without RSO interaction [22,23]. Therefore, we expect that the minimal conductivity of monolayer graphene with RSO interaction shows a similar anisotropic behavior as that obtained for bilayer graphene in Ref. [16].

To see this anisotropic behavior, we calculate the minimal conductivity using tight binding (TB) calculations and compare it to results obtained from a continuum model. We study the effects of finite sample sizes and the crystallographic orientation as well as the length dependent oscillatory behavior of the minimal conductivity. In our two-terminal calculations, the ballistic scattering region of monolayer graphene with length L and width W is contacted by two highly doped regions oriented at angle φ with respect to the zig-zag direction of the graphene lattice (see Fig. 1). Doping in the electrodes is achieved by shifting the Fermi energy with a large potential U_0 as it is commonly done in the literature (see, e.g., Ref. [11]).

2. Landauer–Büttiker formalism for calculating the conductivity

In the Landauer–Büttiker approach the conductance of a sample is given by the transmission probabilities of an electron passing through it:

$$G = \frac{e^2}{h} \sum_{m,n} |t_{mn}|^2, \tag{1}$$

where t_{mn} are the transmission amplitudes between the propagating modes n and m of the left and right electrodes. In what follows, we calculate the minimal conductivity in the TB model (for finite W) and compare the results to that obtained in the continuum model (for $W \to \infty$). Both in TB and continuum models the transmission amplitudes t_{mn} are calculated by solving the scattering problem of the system. Then the minimal conductivity is defined as $\sigma = (L/W)\, G$, with the conductance G calculated from

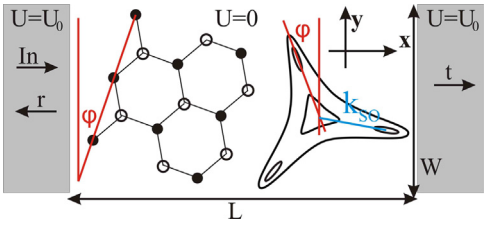

Fig. 1. Geometry of a graphene device of length L and width W between two electrodes doped by potential U_0. Electrons incoming from the left lead are reflected with amplitudes r and transmitted with amplitudes t. Between the two contacts we depict the real space structure of the monolayer graphene flake (left side) and the energy contours in reciprocal space around the **K** point. The zig-zag direction of the graphene flake makes an angle φ with the electrode interface (y direction).

Eq. (1) at the charge neutral point of graphene, i.e., at $E_F = 0$.

2.1. Tight binding model of graphene including RSO coupling

In the TB model the Hamiltonian H_{TB} of monolayer graphene with RSO coupling can be written as [22–25]

$$H_{TB} = H_0 + H_R, \quad \text{where} \tag{2a}$$

$$H_0 = -\gamma \sum_{\langle i,j\rangle,\sigma} (a^\dagger_{i\sigma} b_{j\sigma} + \text{h. c.}), \tag{2b}$$

$$H_R = i\,\lambda \sum_{\langle i,j\rangle,\mu,\nu} \left[a^\dagger_{i\mu} \left(\boldsymbol{s}_{\mu\nu} \times \hat{\mathbf{d}}_{\langle i,j\rangle} \right)_z b_{j\nu} - h.\,c. \right]. \tag{2c}$$

Here H_0 is the Hamiltonian of bulk graphene sheet taking into account only nearest neighbor hopping, with hopping amplitude γ. The operator $a^\dagger_{i\sigma}$ ($a_{i\sigma}$) creates (annihilates) an electron in the ith unit cell with spin σ on sublattice A, while $b^\dagger_{j\sigma}$ ($b_{j\sigma}$) has the same effect on sublattice B and h.c. stands for Hermitian conjugate. The unit cell is given by the unit vectors $\mathbf{a}_1$ and $\mathbf{a}_2$ as shown in Fig. 2. The Hamiltonian H_R describes the Rashba spin–orbit interaction where $\boldsymbol{s} = (s_x, s_y, s_z)$ are the Pauli matrices representing the electron spin, and $\mu, \nu = 1, 2$ denote the $\mu\nu$ matrix elements of the Pauli matrices. Here vectors $\mathbf{d}_{\langle i,j\rangle}$ connect the nearest neighbor atoms $\langle i, j\rangle$ pointing from j to i as shown in Fig. 2, and d is the distance between them, and $\hat{\mathbf{d}}_{\langle i,j\rangle} = \mathbf{d}_{\langle i,j\rangle}/d$ are unit vectors.

The strength of the spin–orbit coupling is denoted by λ which may arise due to a perpendicular electric field or interaction with a substrate.

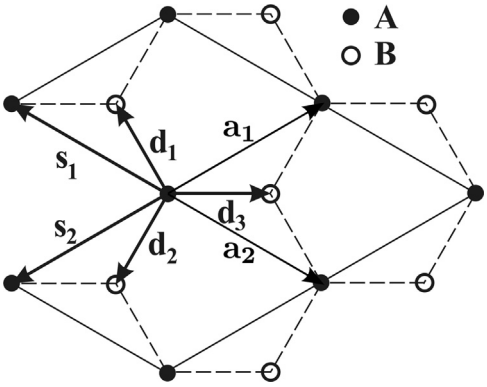

Fig. 2. Geometry of a graphene sheet. The unit vectors of the hexagonal lattice are $\mathbf{a}_1$ and $\mathbf{a}_2$, while $\mathbf{d}_1 = (\mathbf{a}_2 - 2\mathbf{a}_1)/3$, $\mathbf{d}_2 = (\mathbf{a}_1 - 2\mathbf{a}_2)/3$ and $\mathbf{d}_3 = (\mathbf{a}_1 + \mathbf{a}_2)/3$ are vectors pointing to the neighboring atoms.