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Twin lead ballistic conductor based on nanoribbon edge transport

Martin Konôpka *, Peter Dieška

Slovak University of Technology in Bratislava, Faculty of Electrical Engineering and Information Technology, Institute of Nuclear and Physical Engineering, Department of Physics, Ilkovičova 3, 812 19 Bratislava, Slovak Republic

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ABSTRACT

If a device like a graphene nanoribbon (GNR) has all its four corners attached to electric current leads, the device becomes a quantum junction through which two electrical circuits can interact. We study such system theoretically for stationary currents. The 4-point energy-dependent conductance matrix of the nanostructure and the classical resistors in the circuits are parameters of the model. The two bias voltages in the circuits are the control variables of the studied system while the electrochemical potentials at the device's terminals are non-trivially dependent on the voltages. For the special case of the linear-response regime analytical formulae for the operation of the coupled quantum-classical device are derived and applied. For higher bias voltages numerical solutions are obtained. The effects of non-equilibrium Fermi levels are captured using a recursive algorithm in which self-consistency between the electrochemical potentials and the currents is reached within few iterations. The developed approach allows to study scenarios ranging from independent circuits to strongly coupled ones. For the chosen model of the GNR with highly conductive zigzag edges we determine the regime in which the single device carries two almost independent currents.

1. Introduction

Electronic transport through graphene nanoribbons has attracted attention in particular because their zigzag edges exhibit magnetic properties and support specific modes, which may influence the charge transport [1–3]. Edges of larger-scale graphene ribbons have been proposed to serve similarly or analogously to optical fibres or waveguides [4]. In experimental works studying electronic transport through a nanoribbon, the flake is typically contacted to electrodes across its whole width, see for instance Ref. [5]. However, if the edges are to be used for the transport, it may be appropriate to make contacts only to the corners of such a ribbon. This poses a question if a single graphene nanoribbon or an alternative planar atomistic structure could serve as two wires carrying two independent electric currents. Obviously, there would be some interaction between the currents flowing along the two parallel edges and they would not be fully independent. Still, if the energy ranges of the high density of states, resulting from the zigzag (ZZ) edge modes, are used for the transport, the conductance along the ZZ direction may be significantly larger than the conductance along the perpendicular (armchair, AC) direction. In such case the two ZZ edges might be considered as two relatively independent spatially separated conductors. More generally, such scenario would be the case if the 4×4 conductance matrix of a ribbon preferred one of the directions over the perpendicular and diagonal directions. On the other hand, a nanoribbon with significant conductance along several directions would allow to study the intriguing regime in which the two classical circuits are coupled through the quantum ballistic device. Regardless of the conductance characteristics, such setups would naturally require four electrodes contacted to the corners of the nanoribbon.

Electronic transport through graphene flakes with electrodes contacted at their corners has been studied computationally in Ref. [6], with focus on non-rectangular flakes such as trapezoids or triangles. The work has addressed the question how the two-contact conductance qualitatively depends on the magnitude of the angles in the two contacted corner areas and on the types of the edges forming the corner. It was in addition found that the usual nearest-neighbor (NN) tight-binding (TB) model was insufficient for proper description of the edge-induced transport properties (provided that the electrodes were attached to the corners).

Four-terminal phase-coherent conductance has been considered by Büttiker [7] in order to clarify the occurrence of asymmetric magnetoresistances. The author considered a sample contacted to two circuits, what is a setup similar to the one assumed in the present work. On the contrary, the model of Büttiker does not include any classi-

* Corresponding author.
E-mail address: martin.konopka@stuba.sk (Martin Konôpka).

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cal resistors and is limited to the linear regime. We will return to it in the exposition of our theoretical description. Four-terminal schemes have many times been studied both theoretically and experimentally in setups with two voltage probes implying that two of the four terminals carry zero net currents. Analysis of this specific model can be found as early as in the above cited work by Büttiker. A four-terminal electron waveguide coupler was proposed and theoretically analysed in Ref. [8], assuming ballistic transport. Based on the formulae of Ref. [7], Büttiker's resistance tensor of the about 500 Å long junction has been calculated. In Ref. [9] an experimental realisation of two parallel wires coupled by a ballistic window was described. Molecular logic gates with intramolecular circuits are another example of nanoscale multiterminal devices. Considered schemes include both ballistic components as well as classical resistors [10,11]. Theoretical analysis and computational results on multiple-lead coherent conductors in case of finite applied voltages were reported in Ref. [12]. A particularly studied case was a four-terminal conductor with two of the currents set to zero. Voltage difference between the two open leads as a non-linear function of the current was calculated.

In this paper we study a coupled quantum-classical device consisting of a ballistic transport junction and of two classical circuits with the four leads contacted at the junction. As a concrete realisation of the junction a GNR is considered. The two electric currents are driven by DC bias voltage sources in the circuits that include resistors. For the linear regime, transparent analytical formulae displaying the interplay of the quantum and classical elements are derived for both the electric currents as well as for the electrochemical or electrostatic potentials in the device's leads. A numerical scheme is described to tackle the non-linear regime of the composite system. In order to include the effects of the non-equilibrium (NE) electrochemical potentials (EChPs) on the current-voltage characteristics and other quantities, a recursive method for the coupled device is developed. Numerical demonstrations are performed for both a perfect GNR and for a perturbed one. We show that under certain conditions the two electrical circuits of the scheme operate almost independently. Hence such a GNR could serve as two relatively independent conductors, which might be found useful in experimental setups and practical applications as it would allow to shrink the device size. The other regime, in which the circuits are significantly coupled through the ballistic device, presents an interesting physical model and is cover by our numerical demonstrations as well.

In Sect. 2 we define the system under study. In Sect. 3 we derive main results of our work both for the linear and non-linear regimes. We also provide additional description of the studied model, relevant for the NE calculations. In Sect. 4 we apply the theoretical modelling to study the setup defined in Sect. 2. Additional details can be found in the Supplementary Material (SM) [13]. We conclude our results in Sect. 5.

2. The model and methods

2.1. The physical model

An atomistic model of the considered GNRs is shown in Fig. 1. The red-marked carbon atoms in the corners form the contact areas, where the four electrodes (not shown) are attached. If this is accomplished, the whole system in a simple electrical setup can be described by the scheme drawn in Fig. 2. The resistances R_A and R_B of the two classical resistors are known parameters. The control variables are the static bias voltages V_A and V_B on the two DC sources, *not* the EChPs in the leads. The potentials as well as the two currents are unknown non-trivial functions of the bias voltages and have to be determined as it is explained in detail below in the text. The stationary regime is assumed for all elements of the scheme. We consider a low-temperature regime, in which inelastic scattering of the electrons in the GNR and in its contacts can be neglected. Hence the GNR with its contacts represents a quantum subsystem of the entire scheme. The electronic transport properties of such

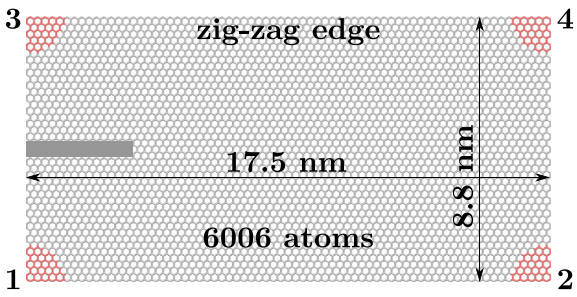

Fig. 1. The graphene nanoribbon (GNR) with the four electrodes attached at its corners, which are labelled as $1, \ldots, 4$ for further reference. Each electrode is modelled by a bunch of 54 identical mono-atomically thin wires [6] (not shown) coupled to the red-marked carbon atoms. The GNR's dimensions are $L = 71\ b$ (along the ZZ edges) and $W = 62\ a$ (along the AC edges), with $a = 0.142$ nm being the nearest-neighbor distance in graphene and $b = a\sqrt{3}$ the lattice parameter. The GNR is composed of 6006 atoms. In an alternative adapted convention [14] the GNR's dimensions are (143,42). The dark narrow strip on the left-hand side parallel to the ZZ edges marks those atoms (60 in total, grouped in 15 4-atom segments) that are removed from the perfect GNR to form the perturbed structure, which is also considered in the text. A detail of a perturbed GNR is shown as the inset of Fig. 3(b). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

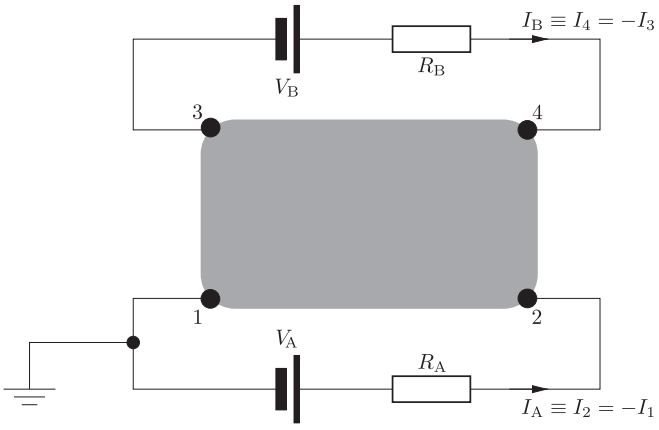

Fig. 2. The electric scheme of the considered device. Given control variables are the two bias voltages V_A and V_B. Additional parameters are the classical resistances R_A and R_B, and the 4×4 conductance matrix G, which in general depends on the energy and on the EChPs of the leads. Stationary regime is assumed for each element of the scheme. The arrows on the leads mark the conventionally positive directions of the currents I_A and I_B in the circuits.

a contacted device in the linear-response regime can be described by a 4×4 conductance matrix G. This matrix is computed using a microscopic model described below. For sufficiently low bias voltages the linear regime with $I_A, I_B \propto V_A, V_B$ can be assumed and the conductance matrix is then considered as energy-independent. This will allow us to derive analytical formulae for currents $I_A(V_A, V_B)$ and $I_B(V_A, V_B)$ in terms of the fixed system parameters G, R_A, and R_B.

We recall that in the scheme under study (Fig. 2), not only the currents but also the EChPs μ_2, μ_3 and μ_4 are unknown non-trivial functions, $\mu_\alpha(V_A, V_B)$, which have to be determined and must strictly be distinguished from the bias voltages. This requirement is dictated by the scheme itself in which the differences $\mu_2 - \mu_1$ and $\mu_4 - \mu_3$ are *a priori* unknown because the currents through the resistors are unknown. The chemical potential at the terminal 1 is fixed by the ground-level condition. One of the foci of the present work is the non-linear response regime with generally non-equilibrium EChPs μ_α in the individual leads. In the non-linear regime, the response of the junction will be described by an energy-dependent conductance matrix $G(\mathcal{E})$ instead just a simple numerical matrix. If, in addition, the NE values of μ_α's are assumed, the conductance matrix will acquire the additional depen-