EFFECT OF CONTACTS ON THE CONDUCTANCE SCALING OF GRAPHENE NANO-RIBBONS

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1. Introduction

Extensive research of graphene was initiated by its unique electronic properties [1] and at the same time by the possibility to prepare graphene samples in laboratories [2]. The dc electronic transport (ET) in ideal graphene and graphene nano-ribbons (GNRs) is of fundamental interest. At energies not too far from the Fermi level, the transport is governed by electrons exhibiting linear dispersion relation which formally bestows them dynamical properties of neutrinos or ultra-relativistic electrons. From band-structure point of view graphene is a zero-gap semiconductor with fully occupied valence band and empty conduction band under charge neutrality conditions. The chemical potential can be altered by a gate voltage and the electronic transport can be studied at its different levels. Intuitively, one might expect zero conductivity at Fermi level. In the experiment by Novoselov, Geim *et al.* [3] the conductivity of graphene was measured as a function of the gate voltage, $\sigma(V_{\rm g})$. It has been found that although the function takes a minimum at zero gate, its value there is non-vanishing, being around $\sigma_{\rm min} \approx e^2/h$. This is the so-called minimal conductivity of graphene. Later Katsnelson [4] and Tworzydło *et al.* [5] calculated its theoretical value $\sigma = \sigma_{\rm min} = (4/\pi)\,(e^2/h)$.

Closely related, the other striking feature of ET in graphene is the classical scaling of its conductance ($G = \sigma\, W/L$) at the neutrality point (zero gate voltage) even in the purely ballistic regime in perfect graphene sheets at low temperatures. This scaling assumes sufficiently wide samples in comparison to their lengths.

Generally, the finite spatial dimensions of GNRs and consequently the boundary conditions must be taken into account in determination of their conductivity. It is known that (ideal) armchair GNRs (AGNRs) can either be metallic or semi-conductive, depending on their width [6, 7]. The zig-zag GNRs are always metallic thanks to their support of special localised states at their edges [6]. Because of the finite size, the conductance in general depends also on the GNR's dimensions L and W. This dependence is non-trivial. It was partially addressed in several works in the past using the Dirac-Weyl model of electrons, see Refs. [4, 5, 8] and it was recently discussed also in our work [9] in order to cover also the range of very narrow and generally very small armchair ribbons for which analytical theories employing the Dirac-Weyl model are not applicable. Briefly, the important findings concerning *perfectly connected*[1] AGNRs are as follows: (i) The ballistic dc conductance G is generally a function of the single variable W/L (as in the classical case) and it is generally a *non-linear* function of the aspect ratio (as opposed to the classical conductance). It may be surprising that this scaling of the conductance is very accurately preserved also for AGNRs as narrow as two carbon rings and/or similarly short. Hence it is sufficient to consider $G = G(W/L)$ and not $G(W, L)$. (ii) For wide-short

[1]The enumerated conductance properties hold if the AGNR is fully coupled to the electrodes, i.e. $t_{\rm GE} = t_{\rm B}$; see below in the text. The electrodes are assumed to be either (semi-infinite) graphene strips or the collections of mono-atomic wires (the model considered in this work).

GNRs ($W/L \gtrsim 4$) the *conductivity* acquires the universal[2] value of $\sigma_{\min}$ (see above). Hence in this Ohmic-like scaling regime it is more practical to use conductivity, rather than the conductance, to describe the ET. (iii) For long-narrow AGNRs ($W/L \lesssim 1$) it is the *conductance* which acquires a constant value of the order $G_0 = 2e^2/h$. In other words, this value is (with very good accuracy) the same for any metallic AGNR satisfying the $W/L \lesssim 1$ condition. Conductivity computed as $\sigma = G_0 L/W$ would of course be dependent on the aspect ratio which is not the case of classical transport. The value of G_0 represents the widely known single conductance quantum (with the factor of 2 coming from the spin degeneracy). The three important characteristics are graphically represented in Fig. 1. Technical details will be explained in Sec. 2.

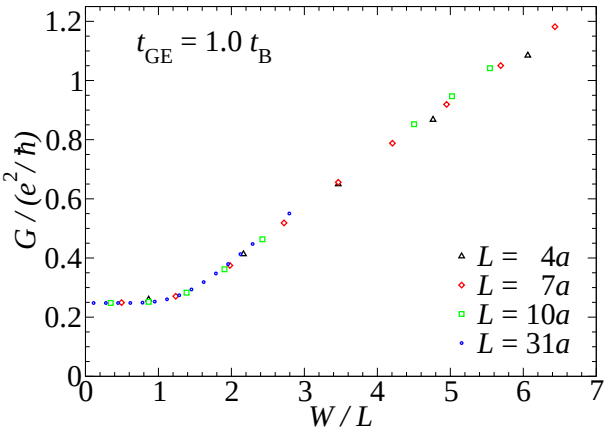

Fig. 1: *Linear conductances of 37 different AGNRs plotted against the AGNRs aspect ratio. The coupling parameter $t_{\rm GE}$ between the AGNRs and the electrodes for this figure is always equal to the bulk coupling parameter $t_{\rm B}$. The AGNRs have four different lengths L shown in legends. (See also Fig. 2.) For the length $L = 4a$ we consider AGNRs of 5 different widths W. Similarly, for $L = 7a$ there are data for 9 widths, for $L = 11a$ we have 8 widths and finally for the longest AGNR ($L = 31a$) we consider 15 different widths. See main text in Secs. 2 and 3 for more details.*

In this contribution we analyse the ballistic conductance scaling with respect to the AGNR length and width for the case when the AGNR is partially isolated form the electrodes via symmetric tunnelling barriers. We have already discussed that the universal $G(W/L)$ dependence becomes lost in this case [9]. It is the purpose of the present contribution to analyse the conductance scaling properties for several different values of the tunnelling barrier and to arrive at conclusions.

2. Description of the studied model

We consider rectangular graphene flakes – nano-ribbons – without any imperfection. One such structure is shown on Fig. 2. The current is assumed to flow in parallel with the armchair edges, hence the name armchair nano-ribbon. This AGNR as well as all other ones considered in this work have the number of dimer lines [6] expressible as $3p - 1$ with p being a whole number. ($p = 10$ for the structure on the figure). This implies the metallic type of AGNR. The shape and symmetry of the other structures considered here is also the same as that

[2] "Universal" is understood here as independent on both W and L or any other parameters.

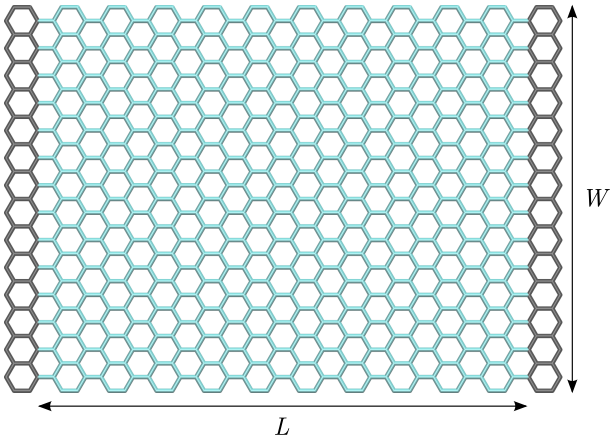

Fig. 2: *One of the considered AGNRs. The dark-coloured strips on the margins represent those atoms to which the electrodes are coupled. The width of the AGNR is* $W = 14\,b$*, with* $b \equiv a\sqrt{3}$ *and* $a \approx 1.42\,\text{Å}$ *being the nearest-neighbour distance in graphene. The total length is* $L_{\text{tot}} = 35a$*. The effective length* L *(which is more important in the present context) is the distance along which the bias voltage is applied and it is* $L = L_{\text{tot}} - 4a$*. The model on the figure contains 696 atoms in total.*

of Fig. 2. They differ by their lengths L and widths W only. The total number of the considered AGNRs is 37. They are of four different lengths: $4a$, $7a$, $10a$, and $31a$. For each length we consider several different widths W such that we cover a wide range of the aspect ratios W/L, both very small and also the cases $W/L > 1$.

Because we consider ET, we have to include electrodes into the total system. The electrodes are modelled here by a set of independent mono-atomic tight-binding wires (chains) which are bonded to the AGNR. The dark colour at the margins of the AGNR on Fig. 2 marks those atoms which are (directly) coupled to the electrodes. The electrons flow from the left electrode to the right one. The described model of the electrodes was used also in Ref. [9]. The inter-atomic separation a between the atoms of the chains is chosen to be the same as in the GNR.

We use the nearest-neighbour tight-binding (TB) description of the whole system with the hopping parameter $t_{\text{B}} < 0$, magnitude of which serves as the energy unit in the present study. The electrons are described in the independent-particle approximation. There is one explicitly considered electron (the $2p_z$ one) per each carbon atom. Such approximation assumes that in real structures the carbon atoms at the edges would have hydrogens attached to saturate the bonds. Although this description is a very basic one, it has proven itself to be surprisingly accurate in the case of graphene.

The TB Hamiltonian for our model is of the standard kind and it has been explicitly introduced in Ref. [9]. We consider only stationary situation (time-independent bias voltage and currents) in the present work. Our focus here is the linear conductance of the AGNRs. We found practical to determine it directly from the formula $G = \lim_{U\to 0} I/U$ in which we use a very small bias voltage $U \ll |t_{\text{B}}|$ and calculate corresponding current I through the system. The stationary currents are obtained from the eigenstate analysis performed using the Green function method [10] in the same way as it was done in Ref. [9].

3. Main results

In Fig. 1 we have reviewed the linear conductances for all of the studied AGNRs in case when the electrodes-AGNR coupling have the full magnitude: $t_{\mathrm{GE}} = t_{\mathrm{B}}$. The conductances are plotted as functions of the aspect ratio W/L. As can be seen, all computed values lie (with a high accuracy) on a single curve which demonstrates that G is a unique function of W/L as said in the introduction. This was a known fact mentioned in a few papers at least for medium-size and larger GNRs [4, 5, 8] although its explicit demonstration covering also very small graphene ribbons was likely missing in the literature until our recent work [9].

We next present the results for the partially decreased GNR-electrodes couplings t_{GE}. The results are shown on Fig. 3 and they have been computed for the same set of AGNRs as used for Fig. 1. They clearly demonstrate that for the reduced coupling the conductance ceases to be a unique function of the aspect ratio only. For a single value of W/L we can have several values of G (belonging to several AGNRs differing by their sizes). Hence for this more general case, G at given value of t_{GE} must be considered as a function of two variables: $G(W, L)$. Another interesting observation acquired by inspection of results in Figs. 1 and 3 is

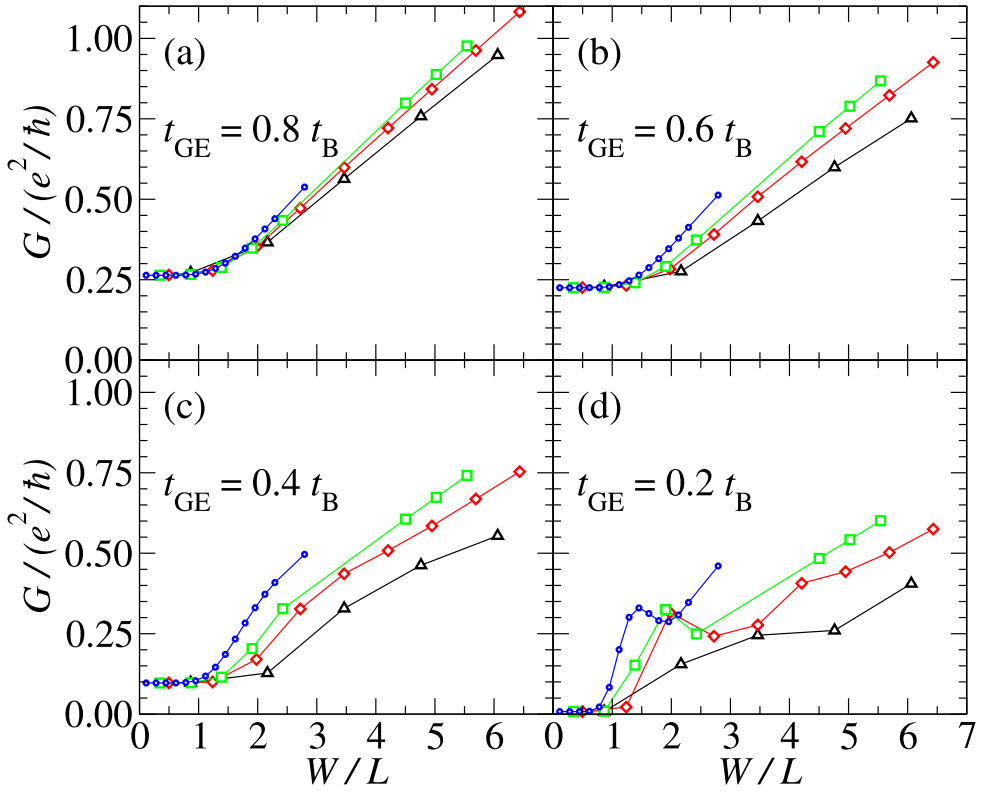

Fig. 3: *Linear conductances of the 37 different AGNRs plotted against the AGNRs aspect ratio. The difference compared to Fig. 1 is that now we consider reduced values of coupling parameter t_{GE} between the AGNRs and the electrodes. They are shown in legends. Otherwise the AGNRs and the colour coding are the same as considered for Fig. 1. The plotted data are strictly functions of the discrete variable W/L. The solid lines used to connect the discrete symbols are just guides for an eye.*

that G for given nano-ribbon may not be a monotonously increasing function of the coupling parameter t_{GE}. For example, the blue plot (represented by the small circles and corresponding to the $L = 31a$ cases) on Fig. 3(d) for $W/L \approx 1.45$ exhibits larger G values than any of the remaining plots for this length, despite the stronger values of t_{GE}, including the plot in

Fig. 1 with the maximum considered coupling. This counter-intuitive behaviour is caused by the reduced impact of the electrodes on the electronic structure inside the nano-ribbons. The partial isolation of the AGNR from its environment causes that environment-induced level shifts and broadenings are partially removed. If there is an electron to be transmitted via such resonant state the resulting transmission amplitude may be increased despite of the smaller tunnelling probability from the electrode to the ribbon.

4. Conclusion

We have performed computational analysis of the conductance scaling of armchair graphene nano-ribbons (AGNRs) with respect to the dimensions of the AGNR for partially isolated AGNR. We have considered AGNRs of the metallic type and the linear conductance at zero gate voltage (the charge neutrality point). While it is known that for such perfectly connected AGNRs the conductance at the neutrality point scales as a unique function of the aspect ratio, $G = G(W/L)$, this is not true if there is a tunnelling barrier between the AGNR and the electrodes. Our tight-binding calculations provided quantitative answers for this prototypical situation. The particularly interesting finding is that even in cases of the partial isolation the conductance is still a unique function of W/L for sufficiently narrow AGNRs ($W/L \lesssim 1$). Another observation is that even a significant partial isolation may, counter-intuitively, increase the conductance.

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