# Transport analysis of graphene-based devices with width discontinuities

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The interest recently raised, in the scientific and industrial community, by graphene electronics has prompted the need for efficient transport simulation codes for graphene-based devices. For relatively large structures, atomistic approaches are too time consuming and it is necessary to resort to a continuum description, based on the solution of the envelope function equation (i.e., for monolayer graphene, the Dirac equation [1]). We have recently proposed a method [2] for the simulation of armchair ribbons in the presence of a generic potential. The ribbon is subdivided into several thin slices within each of which the potential can be considered as constant in the transport direction (a procedure analogous to that we previously adopted for the study of heterostructure-based devices [3]–[7]). In each slice, the Dirac equation can be recast into a problem with periodic boundary conditions [8], which can be efficiently solved in the reciprocal space [2] (or, equivalently, in the direct space using a basis of sinc-related functions [9]), obtaining the longitudinal wave vectors and the transverse components of the envelope functions. Then, the overall conductance is computed applying a scattering matrix approach. In the case of a ribbon with uniform width, the scattering matrices relating couples of neighboring slices are obtained by enforcing the continuity of the components of the wave function on the sublattices $A$ and $B$ along the overall width. In detail, these continuity equations are projected onto a basis of sines extending along the overall width, in such a way as to obtain a linear system in the unknown reflection and transmission coefficients.

Here we describe how this method can be extended to the case of a graphene structure with width discontinuities, made up of several armchair sections.

Generalizing the procedure used to enforce the boundary conditions in armchair and zigzag ribbons [1], we consider the effective boundary of the graphene structure along the lines of lattice sites located just outside the true carbon structure (and represented with dashed circles in Fig. 1). In Fig. 1, with dotted lines we indicate the resulting discontinuities between armchair sections with different width. We notice that the atoms on each of these lines belong to a single sublattice: let us call this sublattice $\alpha$ and the other one $\beta$ (in Fig. 1 $\alpha = B$ along the left discontinuity and $\alpha = A$ along the right one). Each of these lines consists of: (a) zigzag segments of the effective boundary, and (b) segments which instead fall inside the area enclosed by the effective boundary. The conditions we have to enforce are: the vanishing of the only $\alpha$ component of the wave function along the segments (a) (in analogy with the condition imposed at the boundary of a zigzag ribbon [1]), and the continuity of both components of the wave function along the segments (b). Numerically, this can be obtained (in analogy with Ref. [10]) with a scalar projection of the $\alpha$ component of the wave function on a basis of sines of the overall discontinuity, and with a spinorial projection of both components of the wave function on a basis of sines of the segments (b).

As simple examples, in Fig. 3 and in Fig. 5 we report the conductance obtained, following this approach, for the configurations shown in Fig. 2 and in Fig. 4, respectively.

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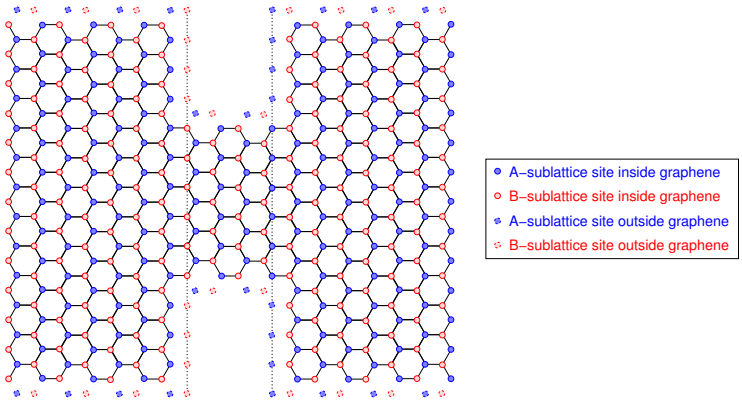


Fig. 1. Schematic representation of the graphene lattice in the presence of width discontinuities.

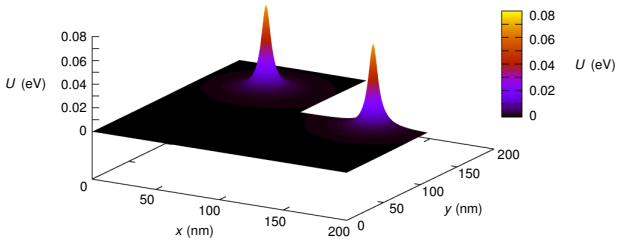


Fig. 2. Graphene structure with a width discontinuity, in the presence of a potential given by the sum of two Lorentzian functions with half-width at half-maximum 4 nm and peak height 70 meV.

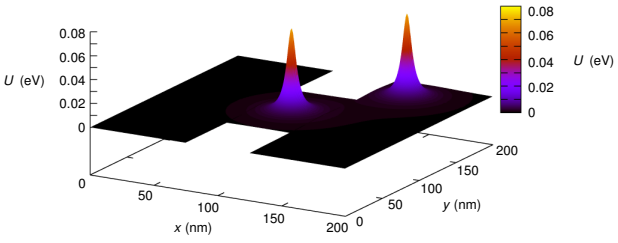


Fig. 4. Graphene constriction, in the presence of a potential given by the sum of two Lorentzian functions with half-width at half-maximum 4 nm and peak height 70 meV.

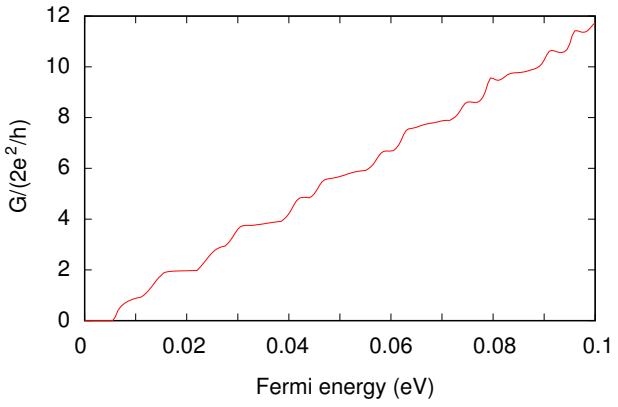


Fig. 3. Conductance behavior, as a function of the Fermi energy, for the structure and potential represented in Fig. 2.

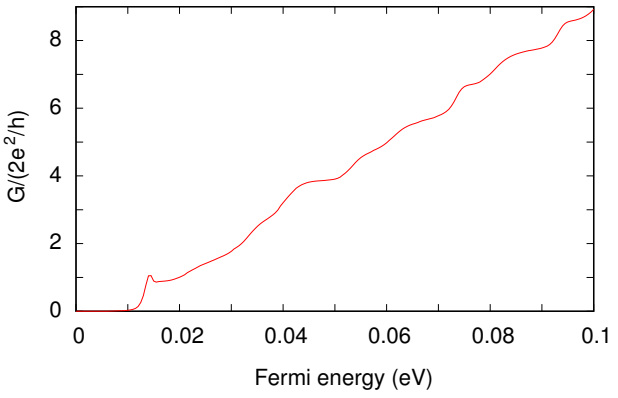


Fig. 5. Conductance behavior, as a function of the Fermi energy, for the structure and the potential represented in Fig. 4.