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Simulation of transport and noise in large-area graphene devices

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We have developed a numerical approach [1] to the efficient and accurate solution of the Dirac equation in graphene samples, with the inclusion of exact armchair boundary conditions. Such an approach allows treatment of relatively large samples, for which an atomistic model (such as tight-binding) would be computationally too demanding, with good accuracy, as long as the potential does not vary too quickly and not too large energies are considered. We have applied our tools to several problems of current interest, such as the calculation of the conductance of a longitudinal device with arbitrary potential landscape, the dependence of shot noise on gate bias in disordered graphene, and the analysis of the dependence on symmetry of the conductance of a double dot.

In Fig. 1(a) we report a sketch of a structure made up of three armchair sections (the one in the center is narrower than the others), in which a potential with two Lorentzians is present. While our method is specifically designed for larger structures, here we focus on a nanometer size one, in order to be able to validate our approach by comparison with the results from a tight-binding calculation. Such a comparison is shown in Fig. 1(b), where a very good agreement is apparent up to an energy of about 0.4 eV, above which there is no interest in a practical device.

In the framework of the investigation of shot noise in disordered graphene, we have applied our technique to samples with a size of hundreds of nanometers (as in the case of the samples studied in actual experiments). Our aim was to understand whether the Fano factor (i.e. the ratio of the measured noise power spectral density to that expected in the case of Poissonian shot noise for the same bias current) depends on gate bias or not, also to explain some experimental results [2]. We report the potential landscape, containing positive and negative Gaussians with an amplitude uniformly distributed between -D and +D, in Fig 2(a), while the results for the Fano factor are shown in Figs. 2(b) (D=0.16 eV) and 2(c) (D=0.5 eV). It is apparent that if a realistic amplitude (0.16 eV) for the potential fluctuations is considered, the Fano factor does depend on gate voltage [Fig. 2(b)], a dependence that disappears only for unrealistic amplitudes [Fig. 2(c)], as in the case of Ref. [3], where, however, only samples with a size of a few nanometers were investigated.

Finally, we present data confirming that also in graphene the conductance of a cavity, connected to the input and output leads by two constrictions and divided into two dots by a potential barrier, depends on the symmetry of the structure (as we have recently observed in semiconductor heterostructures [4]). The investigated device, consisting in a 2 μm×4 μm cavity defined by two 400 nm wide constrictions and with a 30 nm thick and 50 meV high barrier in the middle, is sketched in Fig. 3(a). The computed conductance is shown in Fig. 3(b) as a function of the shift in the position of the barrier with respect to the exact center of the cavity. As we expected, the conductance has a maximum for a symmetric configuration and then quickly drops as we move away from it.

References
Figure 1.
(a) Graphene structure with two 14.9 nm wide armchair regions separated by a 7.5 nm wide armchair section, in the presence of the represented potential energy $U$ (with 2 Lorentzian bumps).
(b) Conductance $G$ (normalized with respect to the conductance quantum $G_0$) as a function of the injection energy $E$, computed with the Dirac equation method (solid curve) and with a tight-binding calculation (dashed curve). The results of the 2 approaches coincide for low energies, where the Dirac equation method is expected to be valid.

Figure 2.
(a) Disordered potential applied to a 200 nm wide and 600 nm long armchair graphene ribbon. The potential is given by the sum of Gaussian functions with a concentration of $5 \times 10^{11} \text{cm}^{-2}$, a half width at half maximum of 10 nm, and an amplitude randomly distributed between -0.16 eV and 0.16 eV.
(b) Fano factor, as a function of energy, for the case represented in (a): the dependence on energy is clear.
(c) Fano factor as a function of energy if the amplitude of the Gaussians is randomly distributed between -0.5 eV and 0.5 eV. In this unrealistic case the dependence on energy is almost completely suppressed.

Figure 3.
(a) Graphene cavity divided into 2 dots by a potential barrier of amplitude $U_0$.
(b) Normalized conductance of the graphene double dot represented in (a), as a function of the longitudinal shift of the potential barrier from the center of the cavity, for an injection energy equal to 30 meV, a 2 µm wide and 4 µm long cavity delimited by 400 nm wide and 250 nm long constrictions, with a 30 nm thick and 50 meV high tunnel barrier. The conductance has a maximum when the barrier is exactly at the center of the cavity.