Numerical simulation of scanning gate spectroscopy in bilayer graphene in the Quantum Hall regime

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Abstract—We propose a model for the numerical simulation of a two-terminal scanning gate spectroscopy experiment on bilayer graphene in the Quantum Hall regime. We start from the Chalker-Coddington random network model and link the model parameters with some of the relevant quantities in the experimental setup. The comparison between the simulation and the measurement results show a good qualitative and in several ways, quantitative agreement.

INTRODUCTION

The Integer Quantum Hall effect (IQHE) is a relevant behavior of two-dimensional disordered electron systems in a strong perpendicular magnetic field. Since its discovery in 1980, it has been attracting significant interest, prompted, on the one hand, by the search for a satisfactory understanding of the physical phenomena involved, and, on the other hand, by the possibility of exploiting the precision in the conductance quantization to define the international standard for resistance in terms of fundamental constants alone.

Actually, there are three known distinct types of IQHE: beside the conventional effect characteristic of (non-intrinsically) two-dimensional semiconductor systems, a second and a third type of behavior have been observed in monolayer and bilayer graphene [1], respectively. The discovery of the IQHE in graphene has paved the way for implementing a new metrological standard at relatively low magnetic fields and even at room temperature, and it has opened the issue of the extent to which the effect in these novel materials shares the same explanation with that in ordinary two-dimensional electron systems.

Here we present simulation results for magnetotransport in bilayer graphene based on a model ini-



Fig. 1. Depiction of a typical disorder potential. The map at the bottom shows the level curves for a value close to the average of the potential. A possible percolating path going across several saddle points of the potential (circles) is highlighted.

tially developed for conventional two-dimensional systems; in order to make a close comparison with experimental data possible, we simulate experiments of scanning probe spectroscopy (SGS), a technique particularly suitable for the investigation of the IQHE, due to the possibility to perturb, with high spatial resolution, the localized states induced by the magnetic field.

MODEL

Although more detailed but complex descriptions, for example tight-binding (as in [2]) or $\vec{k} \cdot \vec{p}$ [3] (as in [4]), can be used, here we adopt a simpler representation of the IQHE as a percolation phenomenon, referring, in particular, to the model proposed by Chalker and Coddington [5], [6], which has proved



Fig. 2. Sketch of the adopted network model: the arrows describe the drift of electrons around the hills (+) and valleys (-) of the potential, while the scattering matrices S and S' characterize the tunnelling at the saddle points. Adapted from [6].

to capture the main physics of Quantum Hall transport. The validity of the model is restricted to twodimensional systems in the presence of a disorder potential V(x, y) and of a magnetic field for which $|l_B \nabla V(x,y)| \ll \hbar \omega_c$, where l_B is the magnetic length, ω_c is the cyclotron angular frequency, and \hbar is the reduced Plank constant. In these conditions the electrons can be semiclassically described as following closed equipotential orbits and tunnelling at the saddle point of the potential, where the orbits get close to each other. In this view, the current can cross the sample only percolating along equipotential paths connecting localized electronic states (Fig. 1). The model describes the system as a regular network, with meshes corresponding to localized current loops circulating around the hills and valleys of the potential, and the nodes corresponding to the saddle points of the potential (Fig. 2).

The scattering properties at each node are described by a 2×2 scattering matrix. As a result of the constraint of unitarity, the matrix is specified by the value of a single real parameter; at the lowest level of approximation, this parameter can be considered dependent only on the difference between the energy of the incident electron and the potential at the saddle point. The network includes two kinds of matrices: their different dependence on the parameter accounts for the different arrangement of the maxima and the minima of the potential around the saddle points they describe. The disor-



Fig. 3. Illustration of the model used to establish a link of the random network model with some of the parameters that can be tuned in the setup of a scanning gate spectroscopy experiment. C_Q is the quantum capacitance (per unit area) at the considered saddle point.

der in the actual spatial distribution of the saddle points is introduced by randomizing the phase shift associated to the paths connecting nearest-neighbor nodes.

We augment this model by taking into account the modulation of the potential U_{ij} associated to the generic saddle point at (x_i, y_j) as a function of the voltage applied to the backgate and to the probe $(V_{BG}$ and V_T , respectively: see Fig. 3) and of the position of the probe. We also include a random fluctuation of the potential in correspondence of the saddle points.

In detail we set $U_{ij} = U_{ij}^{(0)} + \delta U_{ij}$, where $U_{ij}^{(0)}$ is a randomly generated value for each saddle point, and we evaluate δU_{ij} by solving the system obtained coupling the expression for the variation of the local density of charge $\delta \rho_{ij}$ in terms of the voltages applied to the backgate and to the probe with the $\delta \rho_{ij}$ expressed in terms of integrals of the local density of states:

$$\begin{cases} \delta \rho_{ij} = (C_{BG} + C_{T,ij}) \frac{\delta U_{ij}}{-e} - (C_{BG} V_{BG} + C_{T,ij} V_T) \\ \rho_{ij}^{(0)} + \delta \rho_{ij} = \\ + e \int_{-\infty}^{U_{ij}^{(0)} + \delta U_{ij}} DOS(E - U_{ij}^{(0)} - \delta U_{ij}) [1 - f(E)] dE \\ - e \int_{U_{ij}^{(0)} + \delta U_{ij}}^{\infty} DOS(E - U_{ij}^{(0)} - \delta U_{ij}) f(E) dE \end{cases}.$$

We indicated with $\rho_{ij}^{(0)}$ the local density of charge induced by the unperturbed potential $U_{ij}^{(0)}$, and with C_{BG} and $C_{T,ij}$ the coupling capacitances per unit area between the back-gate and the graphene, and the probe and the graphene, respectively. The term e denotes the modulus of the electron charge, while f(E) indicates the Fermi-Dirac occupation factor at the energy E. We model the local density of states LDOS(E) with a sum of Lorentzians centered at the Landau energies of electron motion. We left the broadening of the Landau levels as a fitting parameter, assuming it, as a good approximation in the physical conditions for which the model applies, independent of energy and of the same order of the potential fluctuations [7]. Moreover, we assume that the potential, supposed slowly varying on a length scale of the order of the lattice constant, induces locally in the LDOS a rigid shift in the energy, setting for the generic saddle point of coordinates (x_i, y_j)

 $LDOS_{ij}(E, U_{ij}) = LDOS_{ij}(E - U_{ij})$.

It has been shown by means of self-consistent calculations [8] that the experimental data for the spatial dependence of the charge density induced by the probe can be accurately fitted by the sum of two two-dimensional Lorentzians, with the amplitude linearly dependent on V_T . The higher and narrower of these Lorentzians describes the coupling between the probe tip alone and the graphene, while the lower and wider one accounts for the long-range effects due to the actual structure of the probe. In order to more easily obtain interpretable results, we neglect long-range effects, modeling the dependence of $C_{T,ij}$ on the node coordinates (x_i, y_j) as a single two-dimensional Lorentzian.

The conductance through the network is computed in the Landauer-Büttiker framework, partitioning the network into slices and using a recursive scattering matrix approach for the evaluation of the overall transmission matrix. Starting from the knowledge of the scattering matrix associated to each slice, it is furthermore possible to evaluate the current through each node, and then to derive a map of the current distribution inside the network.

RESULTS

Our simulations refer to a $\approx 2.5 \times 6 \ \mu m^2$ graphene flake deposited onto a highly doped Si



Fig. 4. Simulated conductance as a function of backgate voltage around the n = 1 Landau level. The inset shows the results of the measurements.



Fig. 5. Maps of the modulus of the current density for the values of V_{BG} indicated by arrows in Fig. 4 (the images are ordered for increasing values of V_{BG}); the current injection is from the lower side of the images.

substrate capped with a 300 nm thick SiO_2 layer. The sample is assumed at a temperature of 8 K and biased with a voltage of 10 mV; the intensity of the orthogonal magnetic field is 6.2 T.

We use a rectangular network of 38×76 nodes, corresponding to an average distance between saddle points of ≈ 60 nm. In the transverse direction we enforce Dirichlet boundary conditions, thus assuming perfect reflection from the edges parallel to the current flow. For the two-dimensional Lorentzian function approximating the spatial dependence of the capacitance per unit area between the probe and the flake, we consider a peak value of 0.5×10^{-9} F cm⁻² and a half width at half maximum of 50 nm. The broadening assumed for the Landau levels in the local density of states corresponds to a disorder potential with fluctuations of the order of 10 meV.

We focus on the transition of the measured N-shaped conductance around the n = 1 Landau level (see Fig. 4).



Fig. 6. Comparison between simulated and measured maps of the variation of the conductance for the values of V_{BG} indicated by circles in Fig. 4, and for $V_T = 1$ V.



Fig. 7. Comparison between simulated and measured maps of the variation of the conductance for V_{BG} corresponding approximately to the middle of the percolative riser, and for $V_T = 1$ V and $V_T = 1.5$ V.

In Fig. 5 we show the maps of the modulus of the current density for three values of V_{BG} .

Compared to the measurements, the maps of the probe-induced conductance variation ΔG that we computed for different values of V_{BG} along the riser show a very similar density and intensity of "hotspots", and the same evolution into a less intricate pattern and final disappearance when V_{BG} moves away from the middle of the riser (Fig. 6). Furthermore, holding V_{BG} constant and sweeping V_T , we observe the same tendency of hotspots to grow and merge together (Fig. 7).

CONCLUSION

We performed numerical simulations of SGS experiments on bilayer graphene in the Quantum Hall regime, within a percolation model widely accepted for the description of IQHE in conventional two-dimensional electron systems. We tested the model against experimental data, tuning the free parameters in order to optimize the agreement. The comparison shows that the experimentally detected behavior can be reproduced from a quantitative point of view choosing typical values for the fitting parameters. Our results provide support for the validity of the adopted model for the description of IQHE physics in bilayer graphene.

ACKNOWLEDGMENT

Support from the European Union under the Contract No. 215752 GRAND (GRAphene-based Nanoelectronic Devices) is gratefully acknowledged.

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