

Simplified evaluation of the electrostatic effect of gate voltages on a graphene layer

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In the last few years, significant interest has been focused on carbon allotropes, which (due to their lattice structure [1], [2]) are characterized by peculiar dispersion relations [1]. In particular, several electronic applications have been proposed for graphene [3], exploiting its interesting properties, and a significant numerical effort has been spent on the transport properties of graphene-based devices. A rigorous analysis requires the self-consistent solution of the transport and electrostatic equations [4]. Even though several methods have been proposed for an optimized solution of the transport equation (see, for example, [5]), this self-consistent solution often represents too computationally demanding a procedure, and an approximate evaluation of the potential in graphene, decoupled from the transport problem, is preferable. Here we describe a method which, extending the approach adopted by Das *et al.* [6], allows a simple, albeit approximate, derivation of the effect of the voltage applied to the gates of the device on the potential at the graphene level.

We consider the presence of a quantity $U_0(\vec{r})$ (absent in Das *et al.*), which represents the total potential profile in the device (including also the effect of doping, impurities, and any other possible source) at a given reference bias point, and which is assumed to be known. We define $\rho_0(\vec{r})$ the corresponding superficial charge density in graphene. When the voltages applied to the gates are shifted away from the reference point (for the generic i -th gate, from $V_{G_i,0}$ to $V_{G_i} = V_{G_i,0} + \Delta V_{G_i}$) the potential profile varies by $\Delta U(\vec{r})$ and the charge density by $\Delta\rho(\vec{r})$. For each point \vec{r} of the graphene flake, these variations can be obtained solving the system (at low temperature):

$$\begin{cases} \rho_0 + \Delta\rho = e \int_{E_F}^{U_0 + \Delta U} \text{DOS}(E - U_0 - \Delta U) dE \\ \Delta\rho = \sum_i C_{G_i} \left(\frac{\Delta U}{-e} - \Delta V_{G_i} \right) \end{cases}$$

(C_{G_i} is the geometrical capacitance between the i -th gate and the graphene sheet, E_F the Fermi energy, and e the elementary charge). The first equation (where we have approximated the local density of states through a shift of the density of states by the local value of the potential) gives the relation between the charge and the potential energy in graphene, while the second one describes the electrostatic effect of the gate voltages on the graphene charge. The quantity ρ_0 can be directly obtained setting the variations to zero in the first equation. Substituting the density of states of unconfined graphene $\text{DOS}(E) = 2|E|/(\pi\hbar^2 v_F^2)$ (\hbar is the reduced Planck constant and v_F the Fermi velocity), the system becomes a quadratic equation in ΔU , which can be solved for each point \vec{r} , in order to find the new potential profile $U(\vec{r})$.

For example, considering the case of the device shown in Fig. 1, we set the backgate voltage to zero and we study the effect on the potential profile of a biased probe (located above the flake and at a certain distance from it), simulating its electrostatic action with a geometrical capacitance $C_G(\vec{r})$ which has a Lorentzian dependence on the distance between each flake point and the probe tip [7]. In particular, for an unbiased probe we consider the two different profiles U_0 (consisting of two smooth potential barriers and of a random distribution of Gaussian bumps, as shown in Figs. 2 and 3, respectively) and in both cases we compute the effect of the application of 20 V or -20 V to the probe: results are reported in Figs. 4 and 5.

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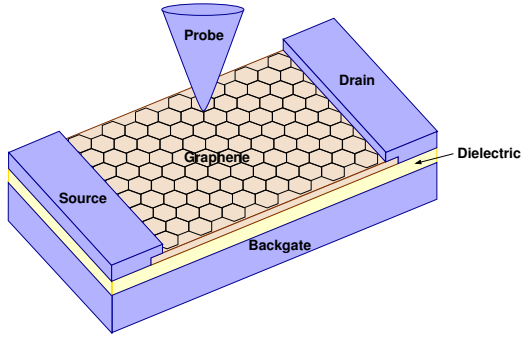


Fig. 1. Device for which we report numerical results.

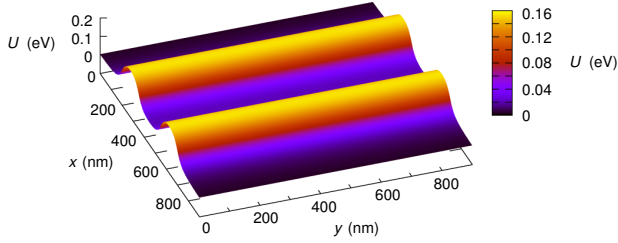


Fig. 2. A profile $U_0(\vec{r})$ that we have considered with an unbiased probe. This potential (consisting of two smooth potential barriers) can result from the electrostatic action of a charge distribution properly deposited over a dielectric on top of the graphene layer.

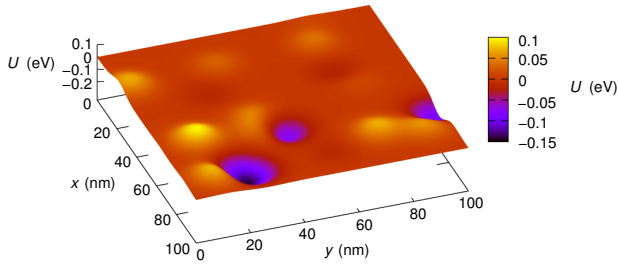


Fig. 3. Another profile $U_0(\vec{r})$ that we have considered when the probe is unbiased. This potential (consisting of 20 Gaussian functions with half-width at half-maximum equal to 7 nm and a peak amplitude randomly distributed between -100 meV and 100 meV) can correspond to the disordered potential commonly present in graphene samples, as an effect of randomly located charged impurities.

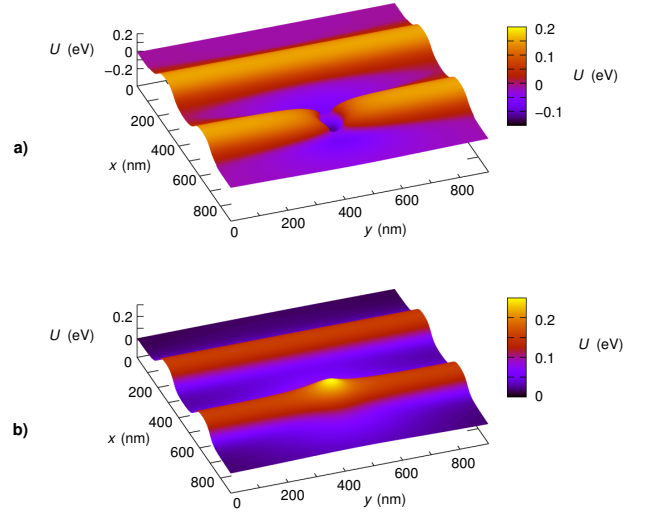


Fig. 4. Graphene potential profile after the application to the probe of a voltage equal to 20 V (panel a) and -20 V (panel b) for the case reported in Fig. 2. The capacitance of the probe $C_G(\vec{r})$ is described as a Lorentzian function (with half-width at half-maximum 50 nm and peak amplitude 0.3 mF/m^2) of the distance between the point \vec{r} and the projection on the graphene flake of the probe position (in this case (625 nm, 450 nm)).

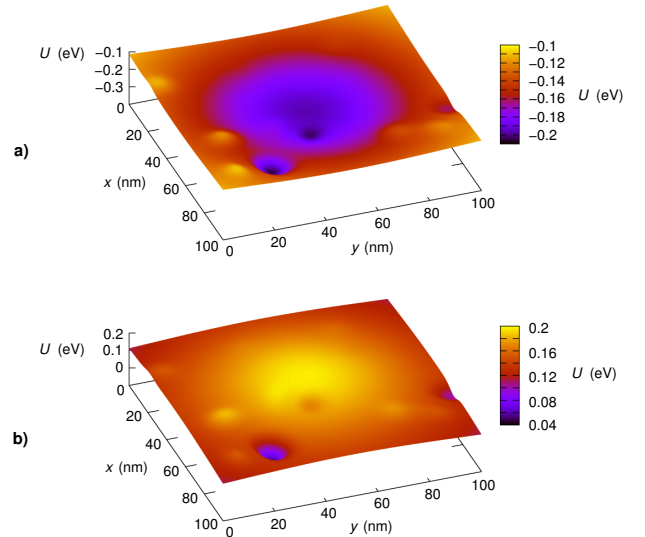


Fig. 5. Effect on the graphene potential profile of the application to the probe of a voltage equal to 20 V (panel a) and -20 V (panel b) for the case reported in Fig. 3. In this case the projection on the graphene flake of the probe position is (50 nm, 50 nm); the other probe parameters are the same as in Fig. 4.