Charge accumulation at the boundaries of a graphene strip induced by a gate voltage: Electrostatic approach

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Distribution of charge induced by a gate voltage in a graphene strip is investigated. We calculate analytically the charge profile and demonstrate a strong (macroscopic) charge accumulation along the boundaries of a micrometers-wide strip. This charge inhomogeneity is especially important in the quantum Hall regime where we predict the doubling of the number of edge states and coexistence of two different types of such states. Applications to graphene-based nanoelectronics are discussed.

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The new material graphene, a monolayer of carbon atoms with honeycomb lattice structure, is attracting a lot of interest since 2005 when the first transport measurements in this material have been reported [1, 2, 3]. The interest in 2D electron gases in graphene originates from the Dirac-like spectrum of the low-energy quasiparticles [4]. Several prominent phenomena have been investigated in this “relativistic” system both experimentally and theoretically, including quantum Hall effect (QH) [5, 6], weak localization and other effects of disorder [7, 8], superconducting proximity effects [9, 10, 11, 12], etc.

In the experiments [1, 2, 3], mechanically exfoliated graphene samples were separated from the metallic gate by a $b \approx 0.3 \mu m$ wide insulating layer ($SiO_2$). The width of the insulator is dictated by the necessity to identify optically the single-layer graphene. In the undoped graphene (half filling), the charge of the conduction electrons is compensated by the charge of the carbon ions forming the lattice. By applying a large ($V_g \lesssim 100 V$) voltage $V_g$ to the lower gate one induces a considerable ($n_e/V_g \approx 7.2 \times 10^{10} cm^{-2}/V$) uncompensated charge $e \times n_e$ in the graphene plane. This extra charge is screened by “image charges” induced in the metallic gate. However, since the images are located $0.6 \mu m$ below graphene, such a screening becomes effective only in the central region of several microns large graphene samples. As a result, the charge distribution cannot be homogeneous.

In this paper, we calculate analytically the charge distribution in the graphene strip and demonstrate a strong increase of the charge density near the strip edges (numerically, a charge accumulation near the edges has been seen in Ref. [13]). For a gate voltage of $\approx 10 V$ the distance between the excess electrons in the sheet is of order $\sim 10 nm$. This means that for the $0.1 \div 1 \mu m$ wide strips one may speak of a continuous charge distribution and determine the latter minimizing the electrostatic energy of the electrons. In semiconductor heterostructures the electron redistribution has been discussed in the context of compressible/incompressible QH stripes formation [14]. However, in that case electrons were confined by a smooth potential, which resulted in a continuous charge density profile at the edge. As we will see, at the sharp graphene edge the charge develops a $1/\sqrt{x}$ singularity.

The charge inhomogeneity discussed in the present paper develops at the scale $\sim 0.1$ micrometer. So this is a macroscopic effect that should have clear experimental consequences. The distribution of classical excess charges found below is valid for any metallic strip. However, only in graphene the excess charge density coincides with the carrier density and determines directly the Fermi momentum, $p_F \propto \sqrt{n_e}$. The charge accumulation at the graphene boundaries is especially important for the quantum Hall effect where we predict coexistence of two types of edge states [14, 15, 16]. The strong dependence of the charge density on the strip width may have interesting nanoelectronic applications, discussed at the end of the paper.

Electrostatic potential created by the charge located on the surface of the insulator, both above and inside,
the potential $E_{\text{ions}}$ may be obtained from the real part of a holomorphic function $w(\zeta)$ as \( \phi = \text{Re} w(\zeta) \), \( \zeta = x + iy \), \( \Delta w(\zeta) \equiv 0 \). In particular, the function
\[
\phi_0 = \frac{4\sigma}{1 + \varepsilon} L(x + iy), \quad L(\zeta) = \text{Re} \ln \left( \frac{\zeta - \sqrt{\zeta^2 - a^2}}{a} \right), \quad (4)
\]
is a solution of the Poisson equation \( \Delta \phi_0 = -4\pi \rho_0 \) with the charge density
\[
\rho_0 = \frac{\sigma}{\pi} \frac{\delta(y)}{\sqrt{a^2 - x^2}}, \quad (5)
\]
where \( \delta(y) \) is the delta-function and \( \sigma \) is the charge per unit length of the strip. The factor \( 2/(1 + \varepsilon) \) in Eqs. (11) accounts for the polarization of the dielectric substrate. The function \( \rho_0 \) is the equilibrium charge distribution, since the potential \( \phi_0 \), is constant on the strip, \( \phi \equiv 0 \) at \( -a < x < a, y = 0 \). The inverse square root edge singularity in Eq. (3) is described by Eqs. (2,3), \( \rho \sim 1/\sqrt{x^2 - a^2} \), drastically differs from the square root density profile \( \rho \sim \sqrt{x} \) at the soft edge in the conventional heterostructures [14].

Straightforward generalization of Eq. (2) gives the potential inside the insulating layer sandwiched between the metallic gate and narrow \((a \ll b)\) graphene strip
\[
\phi = \sum_{n=0}^{\infty} \frac{4\sigma \xi^n}{1 + \varepsilon} \left( \text{Re} \ln \frac{4b}{\varepsilon} \right) \frac{L(\zeta - 2nb) - L(\zeta + 2(n + 1)b)}{1 + \varepsilon}, \quad (6)
\]
Equations (5) and (6) are the central result of this paper describing the charge and potential distributions in the narrow mechanically exfoliated graphene strip. Below we show that these results remain quantitatively accurate even for sufficiently wide strips, when \( a \approx b \).

After the image charges are added the potential on a strip acquires a small, \( \sim (a/b)^2 \), coordinate dependent correction. From Eq. (4) at \( y = 0, -a < x < a \) we find
\[
\phi(x,0) = \frac{4\sigma}{\varepsilon + 1} \left[ \ln \frac{4b}{a} + C_0 + \frac{2x^2 + a^2}{2b^2} C_2 + \cdots \right], \quad (7)
\]
where \( C_0 = \sum_{n=0}^{\infty} \frac{2\xi^n}{1 + \varepsilon} \ln n \), \( C_2 = \sum_{n=1}^{\infty} \frac{\xi^n}{1 + \varepsilon} n^{-2} \). For \( \varepsilon = 3.9 \) we found \( C_0 \approx -0.31 \) and \( C_2 \approx 0.175 \).

The coordinate dependence of the potential Eqs. (6,11) on the metallic strip should be compensated by a proper charge redistribution. Since \( \phi(x) \), Eq. (7), increases towards the edges, one should transfer some charges from the boundaries to the strip center. To find the equilibrium distribution for finite \( a/b \) we add a series of “multipole” corrections to the potential \( \phi_0 \), Eq. (11),
\[
\phi = \phi_0 + \sum_{n=1}^{\infty} \alpha_n \phi_{2n}, \quad \phi_j = \text{Re} \frac{2\sigma(\zeta - \sqrt{\zeta^2 - a^2})^j}{(1 + \varepsilon)a^j}. \quad (8)
\]
The same corrections should be added to all image strip potentials in Eq. (6). Corresponding corrections to the charge density, Eq. (1), are
\[
\rho = \rho_0 + \sum_{n=1}^{\infty} \alpha_n \rho_{2n}, \quad \rho_j = -\frac{1 + \varepsilon}{4\pi} \frac{\delta(y)}{dy} d\phi_j \bigg|_{y=0}. \quad (9)
\]
FIG. 3: Potential (thick lines) and density (thin lines) across  
the strip of width $2a = 2b = 0.6\mu m$. The dashed lines show  
the curves for the density $\rho_0$, Eq. (5) and the solid ones -  
for the density $\rho = \rho_0 - 0.12\rho_2$, Eq. (9). At the plateau one has  
$\phi(x) \approx 0.99\sigma$. A gate voltage $V_g = 100V$ creates in such a  
strip an averaged electron density $(n) = 11.6 \times 10^{12}cm^{-2}$ and  
the minimal density $n(0) = 8.25 \times 10^{12}cm^{-2}$, while an infinite  
graphene plane gives $n_{\infty} = 7.2 \times 10^{12}cm^{-2}$ [1]. Semiclassical  
approximation used for the density calculation breaks at the distance  
$\delta x/b > 0.05(V/V_g)^{2/3}$ from the boundary.  

For example, $\rho_2 = (2x^2/a^2 - 1)\rho_0$. Still the singularity  
$\rho \sim 1/\sqrt{x-a}$ at the edge is generic for any strip width.  

To compensate the $\sim x^2$ term in Eq. (11) it is enough to  
consider the first correction only, $\alpha_2 = -0.175(a/b)^2$.  
This allows us to approximate the equilibrium distribution  
$\phi(x) = const$ with the accuracy better than 0.2% for  
a < 0.5b (strip width $2a < 0.3\mu m$). A simple formula  
(both $V_g$ and $\sigma$ have dimensionality charge/distance)  

$$V_g = \sigma [0.82 \ln(b/a) + 0.88 + 0.29(a/b)^2]$$  
(10)  
relates in this case the linear charge density $\sigma$ in the  
narrow strip to the applied gate voltage.

An appropriate fit with only two parameters $\alpha_2, \alpha_4 \neq 0$  
allows us to reach $\phi(x) \approx const$ on the strip with  
the accuracy $\sim 0.5\%$ even for $a = 5b$ (strip width $2a = 3\mu m$).  
Remarkably, even for such a wide strip the amplitude of  
the $1/\sqrt{x}$ singularity is reduced only by a factor 0.55  
compared to the simple formula, Eq. (10). Fig. 3 shows  
results of the single parameter fit, $\alpha_2 \neq 0$, for $a = b$.  

The classical charges equilibration condition, applicable  
for any metallic strip, allows to find the inhomogeneous  
electron density, Eqs. (5–9), but leads to the constant  
potential in plane. A nontrivial graphene-specific  
potential profile across the strip appears due to quantum  
effects. Quantum dynamics of electrons in graphene is  
described by the Dirac equation  

$$[\nu_F (\tau_x p_x \pm \tau_y p_y) + U(x)]\psi_{\pm} = \varepsilon \psi_{\pm},$$  
(11)  
where $\tau_{x,y}$ are the Pauli matrices interchanging the sub-  
lattice index on the honeycomb lattice. [Strictly speaking  
we should write here $(\tau_x p_x \pm \tau_y p_y)$, since we use coordinates  
x, $z$ for the graphene plane, not $x, y$ used usually in the literature.]  
The two signs $\pm$ correspond to two  

FIG. 4: Schematic charge distribution $\rho(x)$ in units of  
$10^{11}cm^{-2}$ in the QH regime for a strip width $2a = 2b = 0.6\mu m$,  
$B = 10T, V_g = 5V$ (thick solid line). The $\sim 1/\sqrt{x}$  
increase of density at the edge is stopped at $\Delta x \sim l_B = 1/\sqrt{hc/eB} \approx 8\mu m$.  
Short-dashed line shows the electrostatic solution, the same as in Fig. 2.  
We assume valley-degenerate Landau levels, and choose the Zeeman splitting $E_{Zeeman} = 0.25E_0$ [2].  
Lower dashed curves show the effective potential  
for different Landau levels $U_{eff}(x) = U(x) + \sqrt{c n_0} \pm E_{Zeeman}$  
in (units of $0.2eV$). All electronic states with $U_{eff} < 0(> 0)$  
are occupied(empty). Regions with $U_{eff} = 0$ correspond to  
partially occupied Landau levels (compressible stripes).  
The figure shows coexistence of two types of edge states:  
Compressible stripes in the center and usual noninteracting edge  
states at the borders.

valleys in graphene and $\psi_{\pm}$ are envelope functions.  
Solutions of Eqs. (11) are double degenerate due to spin  
and $\nu_F \approx 10^5 cm/s$. The Pauli principle prevents all un-  
compensated electrons in the strip from having the same  
zero momentum, $p = 0$, as was assumed in the electro-  
static solution, Eq. (9). To account for the coordinate  
dependent electron density we introduced in Eq. (11)  
a potential $U(x) < 0$, while keeping the zero Fermi energy,  
$E_F \equiv 0$. For a large charge density, the potential  
$U(x)$ varies slowly on the scale of the wave length $\lambda$,  
which allows us to introduce the local Fermi momentum  
$p_F = h/\lambda_F = |U(x)|/\nu_F$. The density of electrons can be  
found in the Thomas-Fermi approximation as  

$$n_e = 4 \int_{p < p_F} \frac{d^2 p}{(2\pi \hbar)^2} = \frac{1}{\pi} \left( \frac{U(x)}{\hbar \nu_F} \right)^2.$$  
(12)  
The 2-dimensional density of electrons $n_e$ is related to  
the 3-dimensional charge density used in Eqs. (10) as  

$$\rho = e n_e \delta(y).$$  
Thus for narrow strip, $a \ll b$, we find from Eqs. (10)  

$$U(x) = -\hbar \nu_F \sqrt{\pi/e}(a^2 - x^2)^{-1/4}.$$  
(13)  
For the gate voltage $V_g = 100V$ and the strip width $2a = 0.6\mu m$  
we estimate $U(0) = -0.335eV$. This quantum  
$(U(x) \propto h)$ correction to the electrostatic potential on the  
strip describes locally the position of the Dirac crossing  
point with respect to Fermi energy.  

The semiclassical approximation used here is justified  
provided $|d\lambda_F/dx| \ll 1$. Thus we may use Eqs. (5) [13]
only at distances $\delta x > a^{1/3}(e/\sigma)^{2/3}$ from the strip edge. At $\delta x \sim a^{1/3}(e/\sigma)^{2/3}$ the singular increase of both the density Eq. (5) and the potential Eq. (13) is stopped in a way dependent on the details of the graphene edge. In particular, the maximal value of the density is $n_{\text{max}} = \text{const} \times (\sigma^2/e^2a)^{2/3}$ with $\text{const} \sim 1$ depending on the type of the edge.

Experimentally, the conductivity $\Sigma$ of graphene increases linearly with the gate voltage $V$. This implies $\Sigma \propto v_F p_F \propto \sqrt{B}$. The increase of the carrier density near the edges of the strip should lead to an inhomogeneous current density distribution $j(x) \propto \sqrt{\rho(x)}$. Presence of a (moderately strong) disorder should not change the density distribution in the strip.

The non-monotonic charge distribution across the graphene strip should be especially important in the QH regime when the electron transport is due to existence of edge states. The charge density in this case is roughly given again by Eq. (5) with the 1

The energy of the $N$-th Landau level in graphene is

$$E \approx \sqrt{N} E_0, \quad E_0 = \hbar v_F \sqrt{2eB}/hc.$$  

There is a series of such levels for each spin and valley component. So, we find the number of occupied Landau levels at a given point in a strip

$$N(x) = (U(x)/E_0)^2 = n_e\hbar c/4eB.$$  

This formula shows the smoothed number of occupied Landau levels for $N(x) \gg 1$. Going beyond this approximation reveals the compressible and incompressible striped QH states shown in Fig. 4. The picture is schematic since the details of compressible/incompressible stripes are not described by the smooth Eq. (15). Still, this may be done electrostatically, see Ref. [14], in the regions there $dU/dx \ll E_0/l_B$.

The form of the density close to the edge, $\delta x \sim l_B$, as well as the physics of outer edge states, depends on the form of graphene edge. Nevertheless we may say that the lower gate voltage $V_g \approx 5V$ should be sufficient to create several edge states of both kinds for the strip width $2a \approx 0.6\mu m$.

Each QH edge channel supports the electric current flowing only in one direction. For the appropriate sign of the bias voltage $V$, the channel may carry the current $j = e^2V/h$. Since electrons belonging to inner and outer QH edge channels drift in opposite directions, corresponding currents have a tendency to compensate each other. In Fig. 5 we suggest a simple five-terminal device, which would allow to measure separately the currents carried by the outer and inner channels. The QH effect in such a setup would be seen at parametrically smaller values of the gate voltage than in the existing experiments.

A striking consequence of the result, Eq. (14), (see also Ref. [15]) for the strip potential is that for $a \ll b$ the in-plane charge density is inversely proportional to the strip width. (The linear density of charge $\sigma = \int \rho(x)dx$ depends only logarithmically on the strip width, [10], hence $\rho(x) \sim 1/a$). This offers a possibility of creating lakes of a large charge density, quantum dots (QD), by cutting narrow constrictions in the graphene strip. Examples of such devices are shown in Fig. 6. This semi-mechanical way of confining electrons (potentials that appear due to the strip narrowing lead to the longitudinal confinement) may be complementary to the pure electrical way of fabrication of QDs in graphene [22, 23, 24].

Without the electric field doping ($V_g = 0$) graphene behaves as a hole metal [1]. The shift of the Fermi energy away from the Dirac crossing point is attributed to an unintentional doping of the film by absorbed water. It
is compensated by application of a sufficient lower gate voltage ($\sim 40\text{eV}$ [1]). However, as we have shown, the gate-induced charging is nonuniform, and it is impossible by varying $V_g$ to reach the Dirac point simultaneously in the whole sample. This charge distribution evolves differently for $V_g$ below and above the value corresponding to the strip minimum conductivity (for example, the local crossing of the Fermi energy by the Dirac point is shifted towards the center or the boundary of the strip). This may explain the I-V characteristics asymmetry in graphene (observed e.g. in Ref. [12]).

In conclusion, in this paper we predict and describe the macroscopic charge accumulation along the boundaries of graphene strips, made of experimentally used mechanically exfoliated films, for moderate ($\lesssim 10\text{V}$) lower gate voltages. Information about the local Fermi momentum and charge density $p_F \propto \sqrt{\rho}$ may be extracted from the STM measurements of the density of states in graphene [23]. The average charge density ($\rho = \sigma/2a$ for given gate voltage also strongly increases for narrow strips ($\lesssim 0.5\mu\text{m}$) as described by Eq. (10). Transport in graphene would be especially sensitive to the predicted charge accumulation in the experiments [2, 3] in the QH regime, where the two kinds of edge states [14, 13, 10] should coexist in the same sample. Experimental setup capable to measure currents carried by different edge states is suggested (Fig. 5).

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