Quantum Dots in Graphene

P. G. Silvestrov[1] and K. B. Efetov[1,2]
[1]Theoretische Physik III, Ruhr-Universität Bochum, 44780 Bochum, Germany
[2]L. D. Landau Institute for Theoretical Physics, 117940 Moscow, Russia
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We suggest a way of confining quasiparticles by an external potential in a small region of a graphene strip. Transversal electron motion plays a crucial role in this confinement. Properties of thus obtained graphene quantum dots are investigated theoretically for different types of the boundary conditions at the edges of the strip. The (quasi)bound states exist in all systems considered. At the same time, the dependence of the conductance on the gate voltage carries information about the shape of the edges.

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Recently, single layers of carbon atoms (graphene) have been obtained experimentally [1]. This new conducting material with a high mobility [2,3] has attracted a lot of theoretical attention because of its special band structure [4–9]. The spectrum of excitations in graphene consists of two conical bands and is described by a two-dimensional analog of the relativistic Dirac equation.

At the same time, graphene has excellent mechanical characteristics and is able to sustain huge electric currents [1]. One can attach contacts to submicron graphene samples and cut out samples of a desired form and size [1,2]. Applying the electric field one can vary considerably the electron concentration and have both the electrons and holes as charge carriers. Because of these properties the graphene systems look promising for applications in nanoelectronic devices.

One of the most important directions of research using the semiconductor heterostructures is fabrication and manipulations with so called quantum dots that are considered as possible building blocks for a solid state quantum computer [10]. The selection of, e.g., GaAs/AlGaAs for this purpose is related to a possibility of producing electrostatic barriers using weak electric fields. Changing the field configuration one can change the form of the quantum dot, its size, and other characteristics. Considering applications of the graphene systems, the fabrication of quantum dots looks to be one of the most desirable developments in the field.

In this Letter we discuss a method of making quantum dots in graphene strips using *electrostatic* gates. At first glance, the possibility of an electrostatic electron confinement looks surprising since the total density of the conduction electrons is huge $n_e \approx 4 \times 10^{15}$ cm^{-2}. However, the striking feature of the graphene spectrum, namely, the existence of the degeneracy points, makes the local density of the carriers very sensitive to the electric fields. This opens a way to create localized states near the zero energy of the two-dimensional Dirac Hamiltonian.

The existence of bound states in a quantum well is one of the basic features of systems described by the Schrödinger equation. The situation is different for the Dirac equation, since chiral relativistic particles may penetrate through any high and wide potential barriers. This ideal penetration [5–7] means that one cannot automatically transfer to graphene the experience in fabrication of quantum dots in GaAs using the confinement by barriers.

Fortunately, one can still localize the charge carriers in the graphene strip using transversal degrees of freedom of their motion. Moreover, in most of the examples below the mode ideally propagating along the strip is prohibited for the strip of a finite width.

Formation of the quantum dot in a semiconductor wire requires two tunneling barriers. Surprisingly, in graphene it is sufficient to make a single barrier, which may be even simpler from the experimental point of view. The quasibound states exist *inside* the potential barrier, whose left and right slopes work as the ''tunneling barriers'' for the relativistic electrons. The width of the energy levels of these quasibound states falls off exponentially with the width of the barrier and can be very small.

The very existence of the quasibound states (resonances) is independent of the way of the scattering of the electron waves on the edge of the graphene strip (boundary conditions). However, the positions and the widths of the individual resonances and especially the value of the background conductance between the resonances depend on the type of the boundary. Therefore, an experimental realization of our setup would allow one to study properties of the boundary of the real graphene strips.

The electron wave functions in graphene are usually described by a two-component (iso)spinor ψ. Its up and down components correspond to the quantum mechanical amplitudes of finding the particle on one of the two sublattices of the hexagonal lattice. In the absence of a magnetic field, the usual electron spin does not appear in the Hamiltonian and all the electron states have the extra double degeneracy. The Fermi level of a neutral graphene is pinned near two corners $\vec{K}$, $\vec{K}'$ of the hexagonal Brillouin zone, which generates two valleys in the quasiparticle spectrum. The isospinor wave function describing the low energy electron excitations decomposes into a superposition of two waves oscillating with a very different

wave vector $\psi = e^{i\vec{K}\vec{r}}\phi_K + e^{i\vec{K}'\vec{r}}\phi_{K'}$, where $\phi_K = (u_K, v_K)$, $\phi_{K'} = (u_{K'}, v_{K'})$ are two smooth enveloping functions. The latter can be found from the two-dimensional Dirac equation, e.g.,

$$[c(p_x\sigma_x + p_y\sigma_y) + V(x)]\phi_K = \varepsilon\phi_K. \quad (1)$$

Here $c \approx 10^8$ cm/s is the Fermi velocity and $\vec{p} = -i\hbar\nabla$. We consider the graphene strip of the width L placed along the x axis, $0 < y < L$. The smooth potential $V(x)$ is assumed to be created by an external small size gate (tip). We consider the simplest case of a parabolic potential:

$$V = -(x/x_0)^2 U/2. \quad (2)$$

Details of the asymptotics of the potential at $|x| \gg x_0$ are not important for our results. The envelope function $\phi_{K'}$ for the quasiparticle states from the second valley satisfies the same Eq. (1) with replaced sublattice indices, i.e., with $\sigma_y \to -\sigma_y$.

The solution of a couple of two-component Dirac equations (1) in a strip requires a specification of two boundary conditions at each edge of the strip. We first consider the "armchair" edge corresponding to the boundary conditions [8] ($y_{1,2} = 0, L$)

$$u_K|_{y_j} = e^{i2\pi\nu_j}u_{K'}|_{y_j}, \qquad v_K|_{y_j} = e^{i2\pi\nu_j}v_{K'}|_{y_j}, \quad (3)$$

where $i = 1, 2$ and $\nu_1 = 0$. If the graphene strip contains a multiple of three rows of the hexagons, one obtains $\nu_2 = 0$, which corresponds to a metal. Other numbers of rows lead to a semiconducting state with $\nu_2 = \pm 2/3$.

Equations (1) and (2) suggest natural units of length and energy:

$$\xi = [\hbar c x_0^2/U]^{1/3}, \qquad \varepsilon_0 = \hbar c/\xi. \quad (4)$$

In the experiments [1–3], a graphene strip of the width $L \approx 1$ μm was separated by a 0.3 μm thick SiO_2 coating layer from a n^+ doped Si wafer. We expect that the length scale for the potential V, Eq. (2), produced, e.g., by varying the thickness of the insulator layer, or by local chemical doping, is also $x_0 \approx 1$ μm. Assuming also $\xi \approx 1$ μm, we estimate $\varepsilon_0 \approx U \approx 0.66 \times 10^{-3}$ eV. Making the coordinate dependent potential, Eq. (2), of this strength looks rather realistic. For example, reaching the carrier density $n_s = p_F^2/\pi\hbar^2 \approx 10^{12}$ cm^{-2} would require a shift of the Fermi energy away from the half filling by $\Delta E_F = cp_F \approx 0.12$ eV. Even larger carrier densities in graphene were reported in the experiments [2,3].

Solutions of Eq. (1) for the armchair edges have a form

$$\begin{aligned} u_K &= e^{ip_y y/\hbar}(f+g), & u_{K'} &= e^{-ip_y y/\hbar}(f+g), \\ v_K &= e^{ip_y y/\hbar}(f-g), & v_{K'} &= e^{-ip_y y/\hbar}(f-g). \end{aligned} \quad (5)$$

The transverse momentum p_y takes the values

$$p_y(n) = (n + \nu_1 - \nu_2)\pi\hbar/L, \quad (6)$$

where $n = 0, \pm 1, \pm 2, \ldots$. Equation (1) is now replaced by

$$\begin{aligned} [-i\hbar d/dx + V(x)]f - icp_y g &= \varepsilon f, \\ [i\hbar d/dx + V(x)]g + icp_y f &= \varepsilon g. \end{aligned} \quad (7)$$

These equations decouple from each other and can be solved exactly provided the momentum component p_y perpendicular to the strip vanishes, $p_y = 0$,

$$f = e^{iS}, \qquad g = e^{-iS}, \qquad S = \int^x \frac{\varepsilon - V(x')}{c\hbar}dx'. \quad (8)$$

Equation (8) is not what we would like to have because it describes the electron waves propagating *without reflection* along the strip. This is just the $1d$ solution considered previously [5–7]. For $p_y \neq 0$, one cannot solve Eq. (7). However, the *exact* asymptotics at $x \to \pm\infty$ of the solutions has a simple form (8)

$$f_L = e^{iS}, \quad g_L = re^{-iS}, \quad f_R = te^{iS}, \quad g_R = 0, \quad (9)$$

where r and t are two complex numbers, $|r|^2 + |t|^2 = 1$, and the subscripts L, R relate to the asymptotics at $\pm\infty$.

The form of the asymptotics chosen in Eq. (9) corresponds to the electron flux moving from $-\infty$ to $+\infty$, where the coefficient r stands for the reflection and t for the transmission amplitude. The Landauer formula gives the conductance G at zero temperature:

$$G = G_0 \sum |t_n|^2, \qquad G_0 = 2e^2/h, \quad (10)$$

where $t_n = t(p_y(n))$. For the metallic armchair edge, the summation goes over $n = 0, \pm 1, \pm 2, \ldots$, and $|t_n|^2 = |t_{-n}|^2$. The factor 2 in G_0 accounts for the electron spin.

Analytical calculation of the transmission coefficients t_n is possible only for $|\varepsilon| \gg \varepsilon_0$. Figure 1 shows the dependence of the conductance on the Fermi energy ε calculated numerically for $L = 4\xi$ for the metallic armchair strip. At $\varepsilon > 0$ the conductance increases linearly with clearly visible steps $\Delta G \approx 2G_0$ corresponding to the opening of new channels [11]. At negative Fermi energies one can see a series of pronounced resonances. The resonances appear

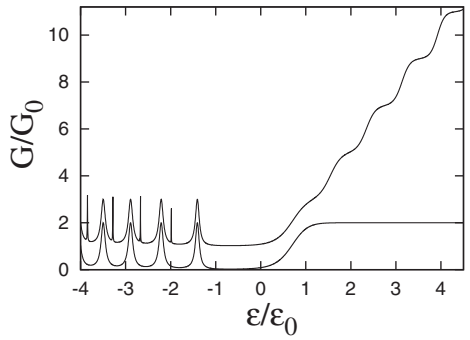

FIG. 1. Upper curve: Conductance of the graphene quantum dot as a function of Fermi energy for the metallic armchair edges for $L = 4\xi$, Eq. (4). Lower curve: Contribution to conductance from the transmission channels with $p_y = \pm\pi\hbar/L$. All calculations are carried out for zero temperature, $T = 0$.

for all nonzero values of the transverse momentum $p_y \neq 0$ (6), but only those corresponding to $|n| = 1$ and $|n| = 2$ are resolved in the figure.

It is easy to understand the reason for the appearance of the (quasi)bound states in graphene. Solutions of the equation $V(x) = \varepsilon$ divide the strip into regions with electron- or hole-type carriers. The lines separating these regions serve as tunneling barriers for all but normal trajectories [6], and this leads to the confinement.

The (semi)classical dynamics of the massless Dirac fermions, Eq. (1), is given by the effective Hamiltonian (see examples of classical trajectories in Fig. 2)

$$H_{\text{eff}} = \varepsilon = \pm c\sqrt{p_x^2 + p_y^2} + V(x). \tag{11}$$

For the (+) sign, particles may either fly freely above the barrier $V(x)$ or start at the infinity and then be reflected from the barrier. The (−) sign in H_{eff} corresponds to the hole solutions of the Dirac equation, whose trajectories bounce inside the barrier for our choice of $V(x)$, Eq. (2). For a given value of the transverse momentum $p_y \neq 0$ four classical turning points where the trajectory changes the direction of the propagation along the strip ($p_x = 0$) are

$$\frac{x_{\text{out}_\pm}}{x_0} = \pm\sqrt{2\frac{c|p_y| - \varepsilon}{U}}, \qquad \frac{x_{\text{in}_\pm}}{x_0} = \pm\sqrt{2\frac{-c|p_y| - \varepsilon}{U}}. \tag{12}$$

The electron coming from the infinity is reflected by one of the outer turning points $x_{\text{out}_\pm}$ if $c|p_y| > \varepsilon$. Thus by changing the energy ε, one changes the number of open channels, which determines the (smoothed) conductance $G \approx 2G_0 L\varepsilon/(\hbar\pi c)$ for $\varepsilon > 0$.

Finite (hole) trajectories bouncing between the two inner turning points $x_{\text{in}_\pm}$ give rise to the quasistationary states. These trajectories appear at $\varepsilon < -c|p_y|$. The position of the Nth resonance ε_N may be found from the quantization rule

$$\int_{x_{\text{in}_-}}^{x_{\text{in}_+}} \sqrt{[\varepsilon_N - V(x)]^2 - c^2 p_y^2}\,\frac{dx}{c} = \pi\hbar\left(N + \frac{1}{2}\right). \tag{13}$$

The resonance acquires a finite width due to quantum tunneling between x_{in} and x_{out}. We can estimate the width using a result of Ref. [6], where the transmission probability through a linear potential was obtained in the form $w = \exp(-\pi c p_y^2/\hbar F)$, where $F = |dU/dx|$ is a slope of the potential. This result can be used in our case provided $c|p_y| \ll |\varepsilon_N|$. Since in this case the interval Δt between the reflections at the points x_{in_-}, x_{in_+} equals $\Delta t = 2(x_0/c)\sqrt{-2\varepsilon_N/U}$, we find the width

$$\Gamma_N = \frac{\hbar}{\Delta t} w = \frac{\hbar v_0}{2x_0}\sqrt{\frac{U}{-2\varepsilon_N}}\exp\left(-\frac{\pi c p_y^2 x_0}{\hbar\sqrt{-2\varepsilon_N U}}\right). \tag{14}$$

Increasing the characteristic length of the potential x_0 we can get extremely narrow levels and long time of the confinement of the electrons in such a quantum dot.

The above results have been obtained for the graphene strip with the metallic armchair edges [$\nu_2 = 0$ in Eq. (3)]. Specific for such edges is the existence of the channel with $p_y = 0$ providing the perfect transmission at any energy $|t_0(\varepsilon)|^2 \equiv 1$. Below we describe the conductance behavior for few other kinds of the edge.

Figure 3 shows the conductance of the semiconductor armchair graphene strip [$\nu_2 = \pm 2/3$ in Eq. (3)] as compared to the conductance of the metallic one, both found from Eqs. (7)–(10). Several striking differences between the two kinds of the edges are clearly seen in the figure. First, since there is no channel with $p_y = 0$, the background conductance around the resonances at $\varepsilon < 0$ vanishes for the semiconductor strip, $G \ll G_0$. In the metallic case the averaged conductance at $\varepsilon < 0$ is $G \approx G_0$. Second, the height of the conductance steps at $\varepsilon > 0$ is $\Delta G = 2G_0$ for the metallic graphene strip and $\Delta G = G_0$ for the semiconductor one. Third, the length of the con-

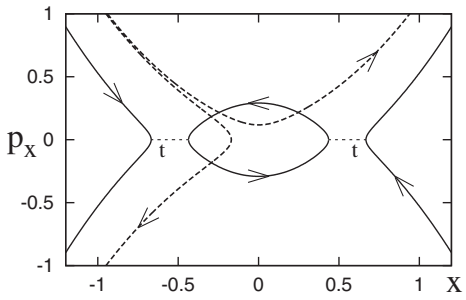

FIG. 2. Examples of trajectories described in the text drawn on the x, p_x plane (arbitrary units). Solid lines show the trajectories with $\varepsilon < 0$ either bouncing inside the barrier or reflected by it from the left or right. Tunneling events between the bounded and unbounded trajectories are shown schematically (t). Thick dashed lines show the trajectories with $\varepsilon > 0$ either transmitted for $|p_y| < \varepsilon/c$ or reflected for $|p_y| > \varepsilon/c$.

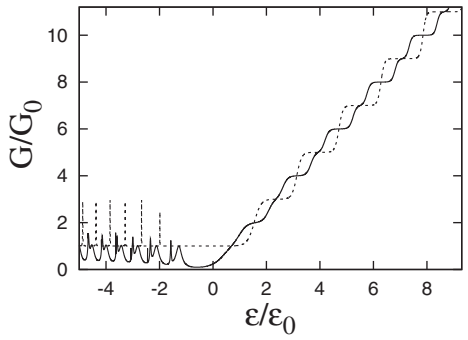

FIG. 3. Conductance of the graphene quantum dot for the semiconductor armchair edge (solid line) compared to the metallic armchair edge (dashed line) for $L = 2\xi$ (4). The nonresonant conductance at $\varepsilon < 0$ is $G \approx G_0$ for the metallic strip and $G \approx 0$ for the semiconducting one. At $\varepsilon > 0$ the conductance steps in the semiconductor case are 2 times smaller, $\Delta G \approx G_0$, and have alternating lengths.

ductance plateaus is constant in the metallic case. On the contrary, the conductance steps in the semiconducting strip have alternating short and long plateaus with $\Delta\varepsilon_2 \approx 2\Delta\varepsilon_1$. In the experiment, one can expect that the metallic and semiconductor strips will be produced in a proportion 1:2.

A way to define the boundary of a Dirac billiard was proposed many years ago in Ref. [12] by introducing an infinite mass for quasiparticle behind the boundary. Reference [9] suggested that in graphene this boundary would correspond to the transverse confinement of carriers by lattice straining. The two (K, K') valleys in this case are decoupled from each other, and one has [13]

$$u_K(0) = v_K(0), \qquad u_K(L) = -v_K(L),$$
$$u_K + v_K = f(x)\cos\frac{p_y y}{\hbar}, \qquad u_K - v_K = g(x)\sin\frac{p_y y}{\hbar}, \tag{15}$$

where the functions f and g are the solutions of Eq. (7). The boundary conditions (15) are satisfied for $p_y = (n + 1/2)\pi\hbar/L$, $n = 0, 1, 2, \ldots$. Each solution, Eq. (15), is fourfold degenerate. Since $p_y \neq 0$, the conductance around the resonances is zero, $G \ll G_0$. The curve $G(\varepsilon)$ looks similar to what we have found for the metallic armchair edges (Fig. 1) but is shifted vertically by $-G_0$.

Another widely considered type of the edge in graphene is the zigzag edge. Since in the case of the zigzag boundary the edges of the strip belong to the different sublattices, the components u and v of the envelope function vanish at the opposite sides of the strip:

$$u_K(0), u_{K'}(0) = 0, \qquad v_K(L), v_{K'}(L) = 0. \tag{16}$$

In addition to the solutions described by the Dirac equation (1), the zigzag edge supports a band of zero energy edge states [14,15]. The (unknown) conductance $\sim G_0$ due to the edge states should be added to the bulk conductance (10). Except for this edge states contribution we do not expect significant differences between the conductance of the strips with the zigzag edges and those confined by the lattice straining [16].

In Figs. 1 and 3 the heights of the resonances are determined by the level of degeneracy (two- or fourfold) of the bound states of the *noninteracting* electrons. In the experiment the shape of the resonances will be governed by the electron *interaction* via the Coulomb blockade effect [17,18]. Since the resonances corresponding to large values of the transverse momentum (14) become exponentially narrow, the multiple charging and repopulation of a broad level introduced in Ref. [19] may occur here.

To conclude, we considered a possibility of localizing charge carriers in a graphene strip by applying an external electrostatic potential. Such a quantum dot can be fabricated using a parabolic potential with a single maximum (minimum). Depending on the position of the Fermi energy, such a device can serve as either a quantum dot or a quantum point contact. The two regimes correspond to either the resonance conductance or the quantized (step-like) one. An experimental realization of our findings would open a way to investigate in graphene the rich physics of individually prepared quantum dots.

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