Landau levels in graphene bilayer quantum dots

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We investigate localized electron and hole states in parabolic quantum dots of biased graphene bilayers in the presence of a perpendicular magnetic field. These quantum dots can be created by means of nanostructured gates or by position-dependent doping, which can create a gap in the otherwise gapless dispersion of a graphene bilayer. Numerical results show the energy levels of confined electrons and holes as a function of the dot parameters and the magnetic field. Remarkable crossings of energy levels are found.

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I. INTRODUCTION

The possibility of the development of carbon-based nanodevices has stimulated a renewed interest in the study of the electronic properties of carbon allotropes, especially since the recent production of single layers of carbon crystals (graphene). These two-dimensional (2D) carbon systems are attractive since they may allow the creation of devices that could benefit from the large charge carrier mobilities and long mean-free paths at room temperature in graphene.[1–5]

Among the striking properties of charge carriers in graphene, their apparent "ultrarelativistic" behavior and a vanishing effective mass result from the gapless and approximately linear spectrum near the Fermi energy at the vicinity of the K and K' valleys in the Brillouin zone. The charge carriers propagate through the graphene honeycomb lattice at a constant "light speed" equal to the Fermi velocity $v_F \approx 10^6$ m/s and are described by the 2D Dirac equation. This massless character of the carriers, together with their chiral nature, is predicted to cause a perfect transmission through wide potential barriers at normal incidence, also known as Klein tunneling,[6–8] an effect that may prevent the electrostatic confinement of charged particles and thus the realization of quantum dots (QDs) in graphene.[9,10] The linear spectrum of electrons in graphene also leads to an unusual quantum Hall effect with the quantum Hall plateaus being found in half-integer multiples of $4e^2/h$. The Landau level (LL) structure of single layer graphene has been investigated by infrared transmission and cyclotron resonance experiments in thin graphite samples[11] and on single layers of graphene.[12]

In contrast to graphene, the spectrum of two coupled graphene layers is found to be approximately parabolic for low energies at two points in the Brillouin zone.[13,14] This is a consequence of the interlayer hopping, which modifies the electronic structure of the system, that nevertheless remains gapless. However, it has been shown recently that the carrier spectrum in bilayers of graphene can be strongly modified by means of chemical doping or by applying an external perpendicular electric field, which breaks the inversion symmetry of the bilayer.[15] This makes it possible to create a tunable gap in the spectrum, which can then be exploited for the development of devices in bilayers of graphene.

One example of such a device is a QD, which can be created by tailoring the electronic structure of a bilayer by means of position-dependent doping or by built-in electrostatic gates in order to create a position-dependent gap, thus allowing the confinement of carriers. Such quantum dots were recently predicted and shown to display new properties not found in conventional semiconductor-based QD.[16] Moreover, the creation of QDs in carbon-based systems can be particularly useful for the development of quantum information applications, due to the long spin coherence times exhibited by electrons in graphene. Bilayers of graphene have been shown to display Landau levels that have an approximate linear dependence on B (Refs. 17 and 18) at low energies, which turns into a $\sqrt{B}$ behavior at higher energies, i.e., high magnetic fields.[19] This behavior has been recently observed in cyclotron resonance measurements.[20] In biased bilayers, however, the Landau level spectrum has been shown to be strongly modified, showing a nonmonotonic dependence on the magnetic field, with the appearance of level crossings as the field increases. In this paper we investigate the eigenstates of localized electrons in a quantum dot created from a graphene bilayer in the presence of a perpendicular magnetic field. We obtain results for the energy levels as a function of the dot parameters and magnetic field.

The paper is organized as follows. Section II gives a description of the model. In Sec. III we show and discuss numerical results. A summary and conclusions are presented in Sec. IV.

II. MODEL

We consider a bilayer of graphene as two honeycomb sheets of covalent-bond carbon atoms in a Bernal AB stacking. The system can be described in terms of two sublattices, labeled A and B (upper layer) and A' and B' (lower layer). The A and B' sites at each layer are coupled via an interlayer hopping term t. In this work we do not take into account possible second-nearest-neighbor terms. Moreover, this calculation describes single electron states. The single electron

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model has been shown to give a reasonably good qualitative agreement with the experimental data so far, although a more precise description should include the effect of electron-electron interactions, as well as other perturbations, such as the interaction with a substrate.[20] The Hamiltonian in the vicinity of the **K** point and in the presence of magnetic field perpendicular to the layer is given, in the continuum approximation, by[21]

$$\mathcal{H} = \begin{pmatrix} U_0 + \frac{\Delta U}{2} & \pi & t & 0 \\ \pi^\dagger & U_0 + \frac{\Delta U}{2} & 0 & 0 \\ t & 0 & U_0 - \frac{\Delta U}{2} & \pi^\dagger \\ 0 & 0 & \pi & U_0 - \frac{\Delta U}{2} \end{pmatrix}, \tag{1}$$

where $t \approx 400$ meV is the interlayer coupling term, $\pi = v_F[(p_x - eA_x) + i(p_y - eA_y)]$, $\mathbf{p}$ is the momentum operator, $\mathbf{A}$ is the vector potential, and $v_F \approx 1 \times 10^6$ m/s is the Fermi velocity. In this work we do not take into account the Zeeman splitting of the energy levels, which can often be neglected for the values of magnetic field considered. The eigenstates of Eq. (1) are four-component spinors $\Psi = [\psi_A, \psi_B, \psi_{B'}, \psi_{A'}]^T$, where $\psi_{A,B}(\psi_{A',B'})$ are the envelope functions associated with the probability amplitudes at the respective sublattice sites of the upper (lower) graphene sheet.

For constant potentials U_1 and U_2, the single-particle spectrum consists of four bands given by

$$E_{\pm}^{+}(k) = U_0 + (1/2)[(t \pm \Gamma)^2 + \Omega]^{1/2}, \tag{2}$$

$$E_{\pm}^{-}(k) = U_0 - (1/2)[(t \pm \Gamma)^2 + \Omega]^{1/2}, \tag{3}$$

with $\Gamma = [t^2 + 4(\hbar v_F k)^2 + 4(\hbar v_F k/t)^2 \Delta U^2]^{1/2}$ and $\Omega = [1 - 4(\hbar v_F k)^2/t^2]\Delta U^2$. For nonzero ΔU the spectrum displays a gap. The existence of such a gap allows the creation of nanostructures based on a position-dependent doping, which in turn can create a position-dependent potential difference between the upper and lower layers of the structure.[22]

Let us now consider a circular-symmetric, position-dependent potential such as the one described in Ref. 16. The carrier states are described by the four-component spinors

$$\Psi(\rho, \theta) = \begin{pmatrix} \phi_A(\rho) e^{im\theta} \\ i\phi_B(\rho) e^{i(m-1)\theta} \\ \phi_{B'}(\rho) e^{im\theta} \\ i\phi_{A'}(\rho) e^{i(m+1)\theta} \end{pmatrix}, \tag{4}$$

where m is the angular momentum label. Using the symmetric gauge $\mathbf{A} = (0, B\rho/2, 0)$, the radial dependence of the spinor components is described, in dimensionless units, by

$$\frac{1}{\sqrt{2}}\left[\frac{d}{d\xi} + \frac{m}{\xi} + \xi\right]\phi_A = (\alpha - \delta)\phi_B,$$

$$\frac{1}{\sqrt{2}}\left[\frac{d}{d\xi} - \frac{(m-1)}{\xi} - \xi\right]\phi_B = -(\alpha - \delta)\phi_A + t'\phi_{B'},$$

$$\frac{1}{\sqrt{2}}\left[\frac{d}{d\xi} + \frac{(m+1)}{\xi} + \xi\right]\phi_{A'} = -(\alpha + \delta)\phi_{B'} + t'\phi_A,$$

$$\frac{1}{\sqrt{2}}\left[\frac{d}{d\xi} - \frac{m}{\xi} - \xi\right]\phi_{B'} = (\alpha + \delta)\phi_{A'}, \tag{5}$$

where $\xi = \sqrt{2}\rho/(2\ell_B)$, $\ell_B = [\hbar/eB]^{1/2}$ is the magnetic length, $\alpha = \epsilon - u_0$ is the energy shifted by the average potential between the layers $u_0 = (u_1 + u_2)/2$, and $\delta = \Delta u/2$, with $\Delta u = u_1 - u_2$. The energy, the potentials, and the interlayer coupling strength are written in dimensionless units as $\epsilon = E\ell_B/\hbar v_F$, $u_{1,2} = U_{1,2}\ell_B/\hbar v_F$, and $t' = t\ell_B/\hbar v_F$. In this paper we will solve Eq. (2) numerically for the case where $U_0 = 0$ and the following parabolic dependence for the potential difference between the layers:

$$\Delta U = \begin{cases} 2U_b(\rho/R)^2 & \rho < R \\ 2U_b & \rho > R. \end{cases} \tag{6}$$

This potential creates a position-dependent gap that vanishes in the center of the QD and which allows the confinement of electrons and holes in the central region, where U_b gives the height of the barriers for both holes and electrons. The smooth position dependence of the potential allows us to neglect intervalley scattering processes, such that the calculation can be carried out separately for each valley. This type of potential profile may be achieved by controlled doping of the surface or by the use of split gates deposited on pristine bilayer graphene.

III. NUMERICAL RESULTS

An unbiased bilayer of graphene displays a $E = 0$ Landau level, as shown in Fig. 1(a), which shows the dependence of the levels on the angular momentum label m, for $B = 5$ T. When the truncated parabolic confining potential given by Eq. (6) is introduced, the degeneracy of the lowest-energy states is lifted, and the resulting spectrum becomes strongly dependent on m, as shown in Fig. 1(b) for a graphene quantum dot of radius $R = 50$ nm, $U_b = 50$ meV, with $B = 5$ T.

For zero external magnetic field, the energy levels of the bound states associated with the QD show a square-root dependence of the potential barrier height (U_b), as depicted in Fig. 2 for $m = -1$ (blue circles), $m = 0$ (black squares), and $m = 1$ (red triangles), for a QD with radius $R = 50$ nm. The results also show the asymmetry between the electron and hole states for nonzero values of m, caused by the breaking of inversion symmetry by the QD potential.

Figure 3 shows results for the spectrum of localized states as a function of the barrier height in the presence of an external magnetic field, $B = 4$ T. As in the previous case, the results are presented for three values of angular momentum

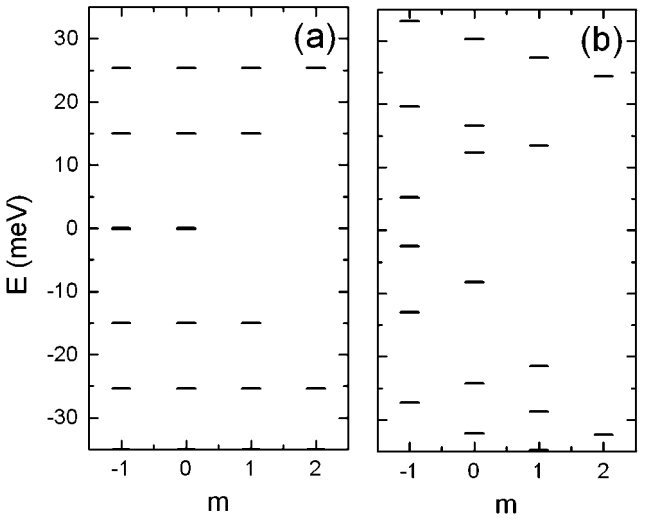

FIG. 1. (a) Landau levels of an unbiased bilayer of graphene as a function of angular momentum label (m). (b) Energy levels of a bilayer graphene quantum dot of radius $R=50$ nm, $U_b=50$ meV. In both cases, $B=5$ T.

label: $m=-1$ (blue circles), $m=0$ (black squares), and $m=1$ (red triangles). For $U_b=0$, the result corresponds to the Landau level spectrum of an unbiased graphene bilayer, with the $m=0$ and $m=-1$ states being degenerate.[19] For small barrier heights, the confinement of the states is mainly caused by the magnetic field. However, as the barrier height increases, the electrostatic confinement becomes important, as seen by the lifting of the degeneracy of the states, and the results approach the $\sqrt{U_b}$ behavior of the previous figure. The $m=1$ branches, in particular, show a strong influence of the field. This comes from the fact that for $m=1$ there are no Landau states with $E=0$,[17] whereas for zero field, the value of the lowest-energy states vanishes as $U_b \to 0$. In addition, for each value of m, the results show some level crossings between energy levels associated with different Landau indices.

Results for the spectrum of localized states as a function of the dot radius are shown in Fig. 4 for $m=0$, U_b

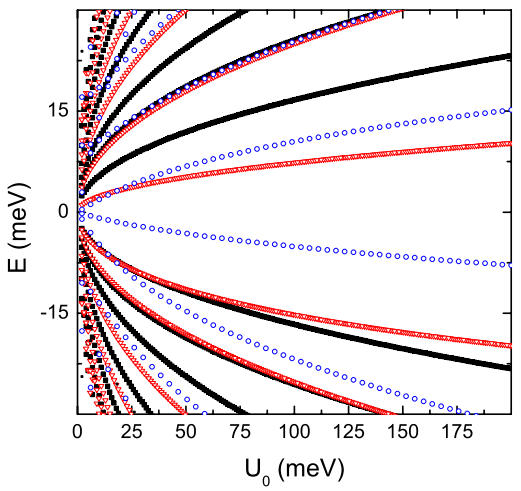

FIG. 2. (Color online) Energy levels of a graphene bilayer quantum dot as a function of the barrier height U_b for $R=50$ nm, $B=0$, $m=-1$ (blue circles), $m=0$ (black squares), and $m=1$ (red triangles).

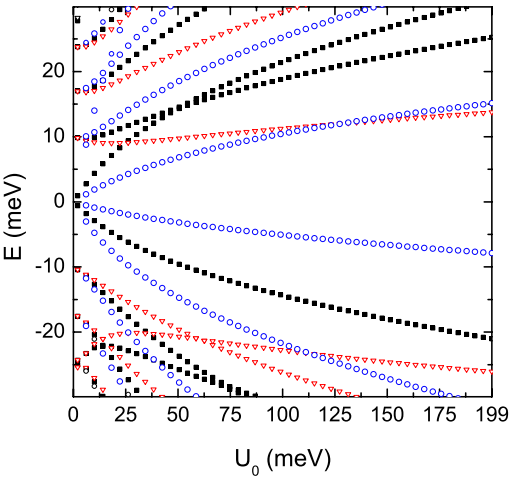

FIG. 3. (Color online) Energy levels of a graphene bilayer quantum dot as a function of the barrier height U_b for $R=50$ nm, $B=4$ T, $m=-1$ (blue circles), $m=0$ (black squares), and $m=1$ (red triangles).

$=50$ meV, $B=0$ T (left panel) and $B=0$, $m=0$ (black dots), -1 (red squares), and -2 (blue triangles) (right panel). For $B=0$, the spectrum shows a $1/R$ dependence. On the other hand, although for nonzero magnetic fields the inverse-radius dependence persists for small radii, as R increases the spectrum becomes weakly dependent on the dot radius, with the energy levels approaching the Landau levels for the unbiased case, for which the $m=0$, $m=-1$, and $m=-2$ states form a set of degenerate levels. One important consequence of the interplay between magnetic and electrostatic confinements is the appearance of level crossings, which occur when states that have lower energy for steeper potentials evolve into magnetically confined states with larger Landau indices. That is a consequence of the nonparabolicity of the band structure of biased bilayer graphene, which displays a mexican hat shape. It is also seen that the low-lying states approach $E=0$, which corresponds to the lowest LL for zero bias. These effects are a consequence of the extra confinement brought about by the magnetic field that, as B increases, tends to

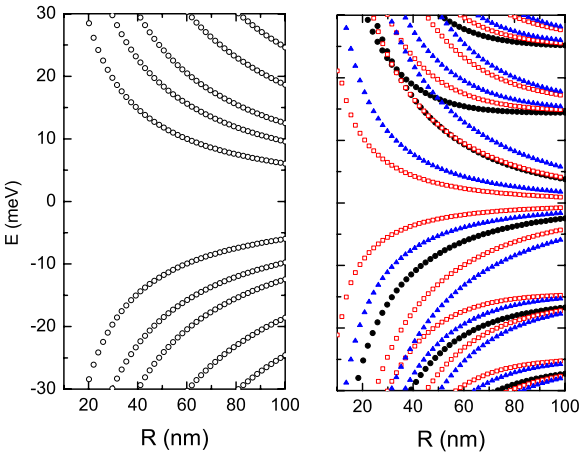

FIG. 4. (Color online) Energy levels as a function of dot radius for $m=0$, $U_b=50$ meV, $B=0$ T, (left panel) and $B=5$ T (right panel).

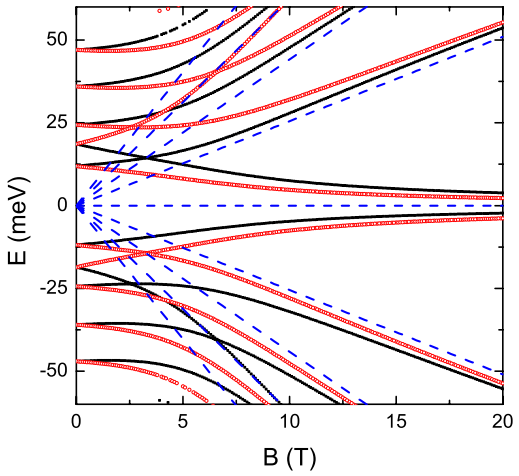

FIG. 5. (Color online) Energy levels in a graphene bilayer quantum dot as a function of external magnetic field with $m=0$ for $U_b=0$ meV (blue dashed lines), and $U_b=50$ meV and $R=50$ nm for both the K valley (black squares) and the K' valley (red circles).

localize the electrons at the vicinity of the origin, where the confining potential is weak. Alternatively, for small values of the confining potential, the eigenstates approach the LL of an unbiased bilayer and as the confining potential increases, it lifts the degeneracy of the LL.

Figure 5 displays results for the energy levels as a function of the magnetic field, for $m=0$, of a quantum dot with $U_b=50$ meV and $R=50$ nm. For large magnetic fields the eigenstates are strongly localized close to the origin, where the potential difference between the layers ΔU vanishes. Therefore, for large values of B, the spectrum approaches those of the Landau levels of an unbiased graphene bilayer, which has an energy state at $E=0$. On the other hand, for zero magnetic field, the energy spectrum of the parabolic quantum dot does not have a zero-energy state. As a result, the field dependence of some electron (hole) energy states displays a negative (positive) slope and approaches $E=0$ as the field increases. That behavior can also be understood by taking into account the fact that as the magnetic field increases, the magnetic length (ℓ_B) becomes much smaller than the dot radius (i.e., for $B=1$ T, $\ell_B \approx 25$ nm, whereas for $B=10$ T, $\ell_B \approx 8$ nm). Therefore, the position of the level crossings can be expected to depend on the dot radius, as well as on the magnetic field strength. The results also show the lifting of valley degeneracy signaled by the splitting of the energy levels associated with the K (black squares) and K' (red circles) valleys. This effect can be explained by the breaking of the electron-hole symmetry caused by the simultaneous presence of a gap and a magnetic field at the barrier region. This breaking of symmetry has been predicted to occur for a *biased* graphene bilayer.[19] As the magnetic field increases, the energy difference between the K and K' states decreases due to the fact that, for larger fields, the magnetic confinement localizes the wave functions in a region of low ΔU. Furthermore, for large values of B the results approach the Landau level spectrum of an unbiased graphene bilayer (dashed blue lines).

IV. CONCLUSIONS

We have obtained results for the energy spectra of confined electrons and holes in quantum dots in bilayer graphene in the presence of a magnetic field. The spectra were obtained from a four-band Dirac-like Hamiltonian that describes the carrier dynamics at the vicinity of the K valley, considering a position-dependent difference in potential between layers which allows the confinement of electrons and holes for zero magnetic field. The results for the spectrum show the effect of the magnetic field on the energy levels of the bound states for different QD parameters, with the results approaching the LL of a uniformly biased bilayer. In particular, the spectra showed the existence of level crossings for several values of magnetic field and dot radii. These crossings are a consequence of the interplay between electrostatic and magnetic confinements together with the unusual electronic dispersion of carriers in a biased bilayer of graphene. These quantum dots may be created by depositing gates on graphene bilayers using lithographic techniques, such as those used previously to investigate transport in graphene nanoribbons, or by means of a controlled deposition of chemical dopants. The energy spectra may be probed by standard spectroscopic techniques, such as the IR cyclotron resonance technique described in Ref. 20, which was employed to investigate the LL structure in unbiased bilayer graphene samples deposited on SiO_2 substrates. Landau levels in single and bilayer graphene have also been previously studied by scanning tunneling microscopy.[23] Such experimental methods can be expected to show the dependence of the intraband transitions energies on the magnetic field and, in particular, the LL crossings.

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