

Graphene quantum dots formed by a spatial modulation of the Dirac gap

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An electrostatic quantum dot cannot be formed in monolayer graphene because of the Klein tunneling. However, a dot can be formed with the help of a uniform magnetic field. As shown here, a spatial modulation of the Dirac gap leads to confined states with discrete energy levels, thus defining a dot, without applying external electric and magnetic fields. Gap-induced dot states can coexist and couple with states introduced by an electrostatic potential. This property allows the region in which the resulting states are localized to be tuned with the potential. © 2010 American Institute of Physics. [doi:10.1063/1.3525858]

The relativistic character of electrons in graphene has attracted considerable attention.^{1,2} This work presents a way of forming a graphene quantum dot as a consequence of a spatial modulation of the Dirac gap.

In an ideal graphene sheet, the band structure has no energy gap and the Dirac electrons are massless. The quantum states of a graphene dot, formed by an external electrostatic potential, are deconfined due to the Klein tunneling that is inherent to massless particles.³ Therefore, an electrostatic dot cannot confine electrons in graphene since these can tunnel through any potential barrier. However, a uniform magnetic field suppresses the Klein tunneling leading to confined states.^{4,5}

It is experimentally possible to engineer an energy gap in graphene's band structure, referred to as a Dirac gap, with a value ranging from a few to hundreds of meV.⁶⁻⁸ The gap leads to electrons with mass and thus an electrostatic potential results in confined states as in common semiconductors.² Most importantly, as shown here, a spatially modulated gap induces confined states regardless of the application of external fields. This can be achieved provided the gap has a local minimum in which the states become localized, thus defining a quantum dot. The application of a potential, generated by a gate electrode, couples the gap and potential-induced states. The coupling strength is tunable with the potential, and it determines the region in which the resulting states are localized.

A spatially modulated Dirac gap has been reported.⁸ Possible ways of creating the required gap modulation that forms the quantum dot include substrate engineering and the application of strain to the graphene sheet.^{1,2}

The physics of a graphene dot, for energies near the Dirac points, is described by the Hamiltonian²

$$H = v_F \boldsymbol{\sigma} \cdot (\mathbf{p} + e\mathbf{A}) + V\mathcal{I} + \tau\Delta\sigma_z, \quad (1)$$

where the Fermi velocity $v_F = \gamma/\hbar$, with $\gamma = 646$ meV nm, is assumed position-independent. $\boldsymbol{\sigma} = (\sigma_x, \sigma_y)$ are the 2×2 Pauli operators acting on the two carbon sublattices, $\mathbf{p} = -i\hbar \nabla = -i\hbar(\partial_x, \partial_y)$ is the two dimensional momentum operator, \mathbf{A} is the vector potential that generates the magnetic field $\mathbf{B} = \nabla \times \mathbf{A}$, V is the electrostatic potential, and \mathcal{I} is the unit matrix. The last term in Eq. (1), referred to as mass term,

gives rise to an energy gap 2Δ in the spectrum of graphene, where $\tau = 1$ ($\tau = -1$) corresponds to the K (K') valley.

For the dot model, V and Δ are chosen cylindrically symmetric and the magnetic field is uniform and perpendicular to the graphene sheet, $\mathbf{B} = B\hat{z}$, so $\mathbf{A} = (0, A_\theta, 0)$, with $A_\theta = Br/2$. The Dirac equation $H\Psi = E\Psi$ can be written in cylindrical coordinates with $\Psi = r^{-1/2}\{f_1(r)\exp[i(m-1)\theta], if_2(r)\exp(im\theta)\}$, where $m = 0, \pm 1, \dots$ is the angular momentum quantum number. The radial functions f_1 and f_2 satisfy

$$(V - E + \tau\Delta)f_1 + \left(U + \gamma\frac{d}{dr}\right)f_2 = 0, \quad (2)$$

$$\left(U - \gamma\frac{d}{dr}\right)f_1 + (V - E - \tau\Delta)f_2 = 0, \quad (3)$$

with $U = \gamma(2m-1)/2r + \gamma eBr/2\hbar$. Equations (2) and (3) are satisfied for both confined and deconfined states. The former have an exponential tail asymptotically, e.g., in the limit of large radial distance $r(r \rightarrow \infty)$, whereas the latter have an oscillatory tail. If for large r V and Δ are constant or have a power-law dependence, then the confined-deconfined character of a state is determined by the asymptotic sign of

$$q(r) = -\left(\frac{eBr}{2\hbar}\right)^2 + \left(\frac{V-E}{\gamma}\right)^2 - \left(\frac{\tau\Delta}{\gamma}\right)^2. \quad (4)$$

A state with energy E is confined only if q is asymptotically negative.⁴ Otherwise the state is deconfined. This criterion indicates that confined states can be induced even for $B=0$ and $V=0$ everywhere, provided that $E^2 - \Delta^2 < 0$ asymptotically. This inequality cannot be satisfied when Δ is spatially independent because all the energies satisfy $|E| > \Delta$. But the inequality can be satisfied when Δ is spatially dependent with an asymptotic value larger than that for small r . This happens, for example, when Δ is zero within a disk area and nonzero outside that area, $\Delta = \delta_0$. Then a number of discrete energy levels satisfy $|E| < \delta_0$ and correspond to confined states with a large amplitude within the disk area. These states can be regarded as dot states.

In the presence of an electrostatic potential V and $B=0$, Eq. (4) shows that if V and Δ are unequal and rise asymptotically, then confined states occur only if $(V-\Delta) < 0$ so that $q < 0$. In this case confinement is energy-independent. How-

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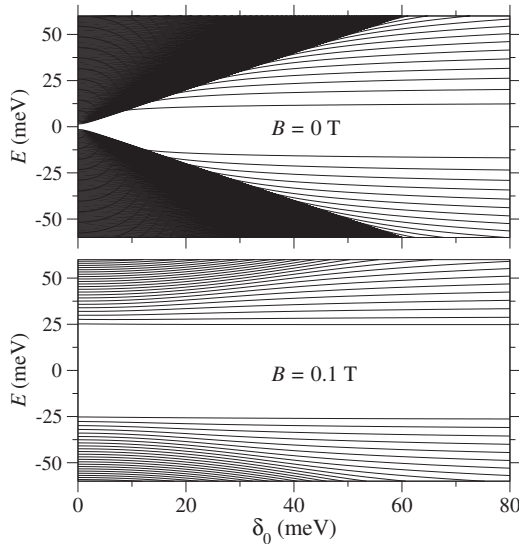


FIG. 1. Energy levels vs the asymptotic value of the mass term δ_0 that generates a Dirac gap $2\delta_0$.

ever, this work focuses on the case where both V and Δ are constant asymptotically, which is the most common experimental regime. Then confinement occurs if $(V-E)^2 - \Delta^2 < 0$ and thus it is energy-dependent.

The properties of the gap-induced dot are analyzed by solving numerically the two coupled equations [Eqs. (2) and (3)] using a discretization scheme, which satisfies time-reversal symmetry: $E(m, B) = E(1-m, -B)$ for $\Delta = 0$ and $E(m, B, \tau) = E(1-m, -B, -\tau)$ for $\Delta \neq 0$. The spatially dependent mass term is modeled by $\Delta = 0$ for $r \leq R$ and $\Delta(r) = -\delta_0 / \cosh[(r-R)/d] + \delta_0$ for $r \geq R$ so that asymptotically $\Delta \approx \delta_0$. This choice is not of particular importance; either a smooth or sharp modulation of Δ results in confined states. For brevity, all the results shown are for $R = 250$ nm, $d = 150$ nm, $\tau = 1$, and $m = 5$.

Figure 1 shows the energy levels as a function of the asymptotic value of the mass term δ_0 for $B = 0$ and $V = 0$. Deconfined states correspond to the (quasi) continuum of levels indicated by the black area in Fig. 1.⁹ Confined states correspond to the discrete levels emerging through the continuum via anticrossing points (see below), forming two distinct ladders of energy separated by a gap. The spacing of the discrete levels and the gap increase with δ_0 . Further, the confinement becomes stronger with δ_0 , and therefore an increase in δ_0 leads to an increase in the number of discrete levels.¹⁰ However, for a fixed δ_0 , not all m values give confined states since the angular momentum term U for $B = 0$ tends to delocalize the states for large m . For this reason there are no confined states for $\delta_0 \leq 10$ meV in Fig. 1. The physics is different if $B \neq 0$ and V is constant since from Eq. (4) $q < 0$ asymptotically, leading to confined states independent of energy. One such case is illustrated in Fig. 1 for $B = 0.1$ T. The continuum of levels has been replaced by a discrete set for all δ_0 , reflecting the disappearance of deconfined states. This is valid for all m values and $\tau = -1$.

The effect of an electrostatic potential on the gap-induced dot is now investigated. The potential that is generated in the graphene sheet by gate electrodes can be calculated within the Thomas-Fermi model.⁴ A slowly varying quantum well potential is approximated by $V(r) = -V_0 \exp$

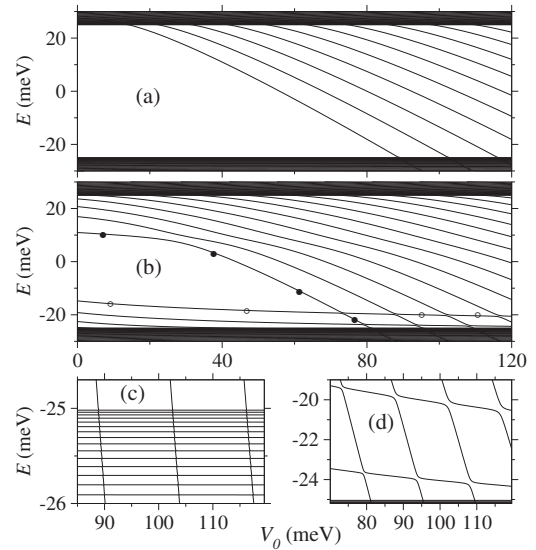


FIG. 2. (a) Energy levels vs the potential depth V_0 for a constant Dirac gap $2\Delta = 50$ meV. (b) As (a) but for a spatially modulated Dirac gap with an asymptotic value of $2\delta_0 = 50$ meV. The states of the energies marked by circles are shown in Fig. 3. Enlarged views of (a) and (b) are shown in (c) and (d).

$(-r^2/l_0^2)$. The quantum well depth is V_0 , the width is l_0 , and asymptotically $V \approx 0$.

Figure 2 shows the energy level diagram as a function of V_0 for $l_0 = 180$ nm. Confined and deconfined states are identified as in Fig. 1. For a constant gap and small V_0 , the angular momentum delocalizes the states; therefore confined states are formed after a critical value of V_0 . The general trend is that with increasing V_0 , the number of discrete levels increases while the lowest levels merge into the continuum. When this happens, the corresponding states undergo a transition from confined to deconfined, which is reflected in the energy diagram by the appearance of anticrossing points [Fig. 2(c)]. These also appear when the states undergo the opposite transition for energies near δ_0 . For a spatially dependent gap, there exist discrete levels even for $V_0 = 0$ because of the gap-induced confinement. Unlike the constant-gap system, as V_0 increases, anticrossing points are formed between discrete levels [Fig. 2(d)], reflecting a coupling between confined states due to the potential and the spatially dependent gap. This coupling is strong for the gap-induced states of the upper ladder of energy and therefore the corresponding anticrossing points are not well-defined. In contrast, states of the lower ladder couple weakly to the potential.

Figure 3 illustrates the effect of the potential on dot states for the energies shown in Fig. 2(b). For $V_0 = 0$, the states are confined owing to the gap modulation. Consider now the states shown in the left panels. As V_0 increases, the gap-induced state with positive energy couples to the potential, e.g., for $V_0 = 30$ meV, and with increasing V_0 it becomes localized in a region defined by the potential. This state then decreases in energy and couples with gap-induced states of the lower ladder, e.g., for $V_0 = 75$ meV. For $V_0 = 120$ meV the state is deconfined with an oscillatory tail, and its energy lies in the continuum. A coupling between gap and potential-induced states occurs also for the states shown in the right panels, e.g., for $V_0 = 75, 120$ meV. As V_0 increases the state with the maximum energy in the lower ladder (for $V_0 = 0$)

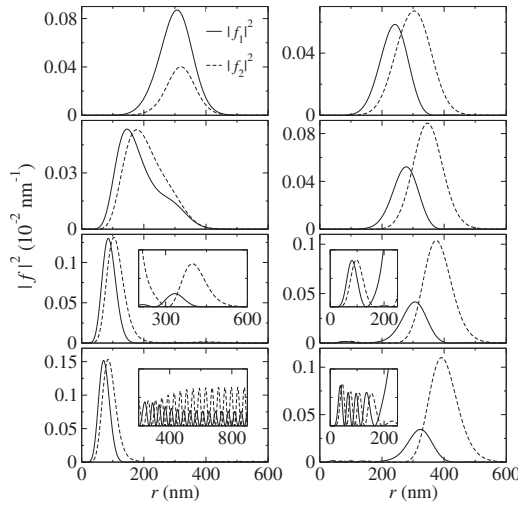


FIG. 3. Quantum states for different potential depths V_0 from top to bottom: $V_0=0, 30, 75, 120$ meV. The Dirac gap is spatially modulated with an asymptotic value of $2\delta_0=50$ meV. Left (right) panels show states with energies marked by \bullet (\circ) in Fig. 2(b). The vertical axes of the insets range from 0 to 2×10^{-3} .

couples with higher excited potential states. This trend is consistent with the series of anticrossing points in the $E(V_0)$ plot.

In Fig. 3 the coupling between potential and gap-induced states of the lower ladder is weak ($V_0=75$ meV); therefore the states peak in the region defined either by the potential profile (left) or the gap modulation (right).¹¹ These two regions have a small overlap when $R > l_0$ and V_0 is large. Strong coupling can be induced for small m ; for instance, for $m=1$ the states peak strongly in both regions. The m -dependence of the coupling can be explained within a semiclassical approach.² The relative maximum amplitude of the two components, as can be derived from Eqs. (2) and (3), satisfies $|f_1| \sim |f_2|$ within a $\Delta=0$ region, whereas $|f_1| > |f_2|$ ($|f_1| < |f_2|$) for energies in the upper (lower) ladder. The latter behavior is more pronounced when Δ is large and constant with $V_0 \neq 0$. Then one of the components becomes vanishingly small depending on the choice of energy and valley ($\tau = \pm 1$).

To probe the states of the gap-induced dot the Fermi level has to be adjusted near the middle of the gap, where only confined states with small values of m lie, and hence the resultant density of states is low. For the same reason the electrostatic potential has to be small. Then, it should be experimentally possible to resolve the quantum states using similar measurements as in GaAs quantum dots.

In summary, a graphene dot can be formed as a result of a spatial modulation of the Dirac gap without applying external fields. An electrostatic potential allows gap and potential-induced states to coexist and become coupled as the potential increases. The coupling strength determines the region in which the states are localized.

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⁹The finite system size leads to a gap at $\delta_0=0$, though it does not affect the discrete levels of the dot.

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¹¹This latter region shifts at larger r with V_0 , and does not bind for a too large V_0 .