Proposal for a magnetic field induced graphene dot

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Abstract. Quantum dots induced by a strong magnetic field applied to a single layer of graphene in the perpendicular direction are investigated. The dot is defined by a model potential which consists of a well of depth $\Delta V$ relative to a flat asymptotic part and quantum states formed from the zeroth Landau level are considered. The energy of the dot states cannot be lower than $-\Delta V$ relative to the asymptotic potential. Consequently, when $\Delta V$ is chosen to be about half of the gap between the zeroth and first Landau levels, the dot states are isolated energetically in the gap between Landau level 0 and Landau level -1. This is confirmed with numerical calculations of the magnetic field dependent energy spectrum and the quantum states. Remarkably, an antidot formed by reversing the sign of $\Delta V$ also confines electrons but in the energy region between Landau level 0 and Landau level +1. This unusual behaviour gives an unambiguous signal of the novel physics of graphene quantum dots.

1. Introduction

Graphene is an astonishing material with a zero energy gap and massless charge carriers. This allows relativistic physics to be studied in the solid state and leads to many remarkable phenomena ¹. One of the most relevant to graphene dots is the quantum Klein paradox. This makes all potential barriers perfectly transparent to graphene charge carriers moving in one and two dimensions ² so it is impossible to confine graphene carriers in an external potential well. However it is possible to confine them with a combination of electric and magnetic fields. Essentially, the magnetic field deflects the carriers so that they move in closed orbits and remain localised but this kind of confinement cannot be achieved with an arbitrary combination of electric and magnetic fields. The conditions needed have been analysed by Giavaras, Maksym and Roy ³ who have suggested a device structure that can be used to probe both confined and deconfined states in graphene dots. The present work is about a simpler structure that can be used to focus on confined states.

Conditional confinement is the one of the most important differences between graphene and conventional semiconductors. It is a direct consequence of the lack of mass. Roughly speaking, confined quantum states occur only when all the corresponding classical orbits are bounded but when massless particles move in a weak magnetic field both bounded and unbounded orbits occur at the same energy. Raising the magnetic field removes the unbounded orbits and enables confined states to occur. Details are given in ref. ³ for circularly symmetric scalar potentials.

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$V = V_0 r^s$ and azimuthal vector potentials, $A_\theta = A_0 r^t$, where $r$ is the radial distance and $s,t > 0$. In this case all the states are confined when $t > s$ but when $t = s$ the states are confined only when $c^2 e^2 A_0^2 > V_0^2$, where $c$ is the Fermi velocity of the graphene sheet. Since $V_0$ and $A_0$ are experimentally tunable parameters this allows both confined and deconfined states to be probed in graphene dots and the interesting transition between the two regimes that occurs when $c^2 e^2 A_0^2 = V_0^2$ could also be probed experimentally.

Another important difference between graphene and conventional semiconductors is that graphene is gapless. Dots in conventional semiconductors are engineered so that the dot states are both confined and have energies in the band gap. Thus the dot states are spatially and energetically isolated from the rest of the system. The dot is an artificial atom and any probe of energy levels in the gap, for example charging experiments, is only sensitive to dot states and does not respond to bulk states. It is more difficult to achieve this in graphene because there is no natural gap. One option is to engineer a device structure that puts confined dot states in the gap between bulk Landau levels. However there is a problem. The potentials in a real graphene dot cannot rise indefinitely as a power law and must become flat asymptotically. So there are bulk Landau states outside the dot and it is necessary to ensure that the confined dot states occur in a region of low density of states away from the broadened bulk Landau levels. Giavaras, Maksym and Roy [3] showed that it is possible to achieve this while allowing the confinement-deconfinement transition to be observed provided that the scalar potential consists of a well which is separated from the asymptotic region by a barrier. However the barrier is not needed if one only wants to probe confined states. Then one can use a simple potential well as shown in figure 1.

A well in a uniform, perpendicular magnetic field clearly satisfies the confinement condition when the field is strong enough. The reason why it also satisfies the condition for energetic isolation is related to the unusual physics of the zeroth Landau level in graphene. In brief, the zeroth Landau level has zero energy and when a potential well of depth $\Delta V$ is applied to graphene the energy of states formed from the zeroth Landau level does not shift by more than about $|\Delta V|$. So dot states can be isolated energetically by choosing $\Delta V$ to put them into the middle of the Landau gap. The same result applies to antidot states, which are also confined because of the symmetry of the Dirac cone. So observations of the symmetry between dot and antidot confined states would give a direct experimental confirmation of the influence of the Dirac cone on the graphene dot energy spectrum. This physics is detailed in section 2 and numerical studies of the dot energy spectrum and quantum states are reported in section 3 where the properties of the graphene dot are compared with those of a typical electrostatic dot formed from GaAs.

2. Physics of Electron Confinement in the Zeroth Landau Level

The graphene sheet is taken to be in a uniform, perpendicular magnetic field, $B$ and the azimuthal component of the magnetic vector potential at position $r$ is $A_\theta = Br/2$, where $\theta$ is the azimuthal angle. The scalar potential is taken to be $V(r) = \pm(V_0 \cos(\pi r/2R) + V_1), r < 2R, V(r) = \pm(V_1 - V_0), r \geq 2R, \quad V_0, V_1 > 0$, where the + sign corresponds to an antidot, the − sign corresponds to a dot and $R$ is a size parameter. In terms of these parameters the depth of the dot and height of the antidot are given by $|\Delta V| = 2V_0$. Because the solution to the Laplace equation can be written as a Fourier series, this simple form is a crude model of the potential in a real dot.

The potentials have circular symmetry so the quantum states are eigenstates of angular momentum, $\hbar m$, where the angular momentum quantum number is the integer $m$. The graphene states are two-component states where each component gives the probability amplitude for an electron being on one of the two sub-lattices of the graphene sheet. The two-component envelope
function is \((\chi_1(r)\exp(i(m - 1)\theta), \chi_2(r)\exp(im\theta))\) and the radial functions, \(\chi_i\) satisfy

\[
\frac{V}{\gamma} \chi_1 - \frac{d}{dr} \chi_2 - \frac{m}{r} \chi_2 - \frac{ie}{\hbar} A_\theta \chi_2 = \frac{E}{\gamma} \chi_1, \\
-\frac{d}{dr} \chi_1 + \frac{(m - 1)}{r} \chi_1 + \frac{e}{\hbar} A_\theta \chi_1 + \frac{V}{\gamma} \chi_2 = \frac{E}{\gamma} \chi_2,
\]

where \(\gamma = 646 \text{ meV nm}\) and \(E\) is the energy. The Fermi velocity is given by \(c = \gamma/\hbar\).

When \(V = 0\) these equations give the graphene Landau levels of energy \(E = \pm \gamma \sqrt{2N}/l\) where \(l^2 = \hbar/eB, \ l\) is the magnetic length, \(N = n + (|m| + m)/2\) is the Landau quantum number and \(n\) is a radial quantum number. The zeroth Landau level states correspond to \(n = 0\) and \(m \leq 0\). Unlike the situation of a particle with mass, the energy of the zeroth Landau level is exactly zero and there is no zero point energy. In addition \(\chi_1\) vanishes and \(\chi_2 \propto r^{|m|}\exp(-r^2/4l^2)\) so that the quantum states are localised on rings whose radius increases like \(\sqrt{|m|}\).

Now consider what happens to the zeroth Landau level states in the presence of a non-zero potential. In this case \(\chi_1\) no longer vanishes but it can be shown that the zero point energy remains small. Consequently the energy of the states is determined mainly by the local potential. In the case of a dot the lowest energy states are those of smallest spatial extent so if the dot is large enough that the \(m = 0\) state fits into it, the energy of the lowest state in the dot is no more than \(\Delta V\) below the asymptotic value of the potential. When \(m\) increases the states are localised in regions of weaker potential so their energy tends to increase with \(m\). In the limit of very large \(m\), the states merge into the bulk zeroth Landau level which is shifted from zero by the asymptotic value of the potential. These statements can be proved rigorously but the details are quite complicated. This physics is the key to isolating a confined dot state energetically.

If \(\Delta V\) is chosen to be about half of the gap between Landau level 0 and Landau level -1, that is \(\Delta V \sim \gamma/4\), the lowest dot state will be in the desired region of very low density of states.

To analyse the case of an antidot consider what happens when \(V\) is replaced by \(-V\). It can be shown by direct substitution into the radial equations that if \((\chi_1(r)\exp(i(m - 1)\theta), \chi_2(r)\exp(im\theta))\) is an eigenstate of energy \(E\) corresponding to potential \(V\), then \((\chi_1(r)\exp(i(m - 1)\theta), -\chi_2(r)\exp(im\theta))\) is an eigenstate of energy \(-E\) corresponding to potential \(-V\). Hence the antidot states are confined whenever the dot states are confined and the energy of the highest antidot state is no more than \(\Delta V\) about the asymptotic value of the antidot potential. The fact that both dots and antidots confine electrons is unique to graphene and is an observable consequence of its Dirac cone band structure.

3. Numerical Studies of Dots and Antidots
To compute energies and states, the radial equations are made real by putting \(f_1 = \chi_1, \ i f_2 = \chi_2\), then \(f_1\) and \(f_2\) are found with the method outlined in ref. \(3\). The model parameters are \(V_0 = 20\) meV, \(V_1 = 30\) meV and \(R = 100\) nm. Hence \(\Delta V = 40\) meV, about half the Landau gap at
5 T and $V(r)$ becomes $\pm 10$ meV outside the dot or antidot. Magnetic field dependent energy spectra are shown in figure 1. Each spectrum consists of a superposition of energy levels and the $m$ range, $-150 \leq m \leq 10$, is chosen so that all states localised in the dot or antidot are included in the field range between 1 and 5.5 T. For comparison, the dashed lines show the Landau levels of an ideal graphene sheet. These levels are shifted by the asymptotic value of the potential, $-10$ meV in the case of the dot and $+10$ meV in the case of the antidot. The effect of the external potential is clearly to broaden the Landau levels. In the case of the dot, the zeroth Landau level at $-10$ meV is broadened into a band that occupies the region between $-10$ and $-50$ meV and the width of the band is very insensitive to the magnetic field. As expected the width of the band simply reflects the range of potential values: no zeroth Landau level state rises in energy above $-10$ meV and no zeroth Landau level state falls in energy below about $-50$ meV. In contrast, the upper edge of the broadened $N = -1$ Landau level falls in energy like $-\sqrt{B}$ and the lower edge of the broadened $N = +1$ Landau level rises in energy like $+\sqrt{B}$. Therefore the band of $N = 0$ dot states becomes energetically isolated as the field increases. With the present model parameters, the lowest dot state appears about in the middle of the gap when the field is about 5 T. In a real graphene sheet the Landau levels are broadened because of imperfections but the same principle applies and the magnetic field and potential can be chosen so that the lowest dot state lies in a region of extremely low density of states between broadened Landau levels. The right hand side of figure 1 shows the antidot spectrum. It has the same features as the dot spectrum except that the band of confined antidot states appears in the gap between the $N = 0$ and $N = 1$ Landau levels. The symmetry between the dot and antidot spectra is clearly visible. Figure 2 shows the lowest ($m = 0$) state in a dot and demonstrates that it is confined within the dot.

![Figure 2](image_url)

**Figure 2.** Two component radial envelope function for the $m = 0$ state in a dot.

In summary, the proposed graphene dot is able to confine electrons in a region that is isolated both spatially and energetically. The typical spacing between the dot levels at $B = 5$ T ranges from $\sim 0.6$ meV for $R = 100$ nm to $\sim 2$ meV for $R = 50$ nm. These sizes and level spacings are comparable to those for a GaAs electrostatic dot with confinement energy 4 meV in a magnetic field range of 3-10 T. The energy levels in the GaAs dot can be resolved by charging experiments, for example, so similar experiments on the graphene dot should be feasible.

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