States near Dirac points of rectangular graphene dot in a magnetic field

S. C. Kim$^1$, P. S. Park$^1$, and S.-R. Eric Yang$^{1,2,*}$

$^1$Physics Department, Korea University, Seoul Korea and

$^2$Korea Institute for Advanced Study, Seoul Korea

(Dated: January 8, 2010)

In neutral graphene dots the Fermi level coincides with the Dirac points. We have investigated in the presence of a magnetic field several unusual properties of single electron states near the Fermi level of such a rectangular-shaped graphene dot with two zigzag and two armchair edges. We find that a quasi-degenerate level forms near zero energy and the number of states in this level can be tuned by the magnetic field. The wavefunctions of states in this level are all peaked on the zigzag edges with or without some weight inside the dot. Some of these states are magnetic field-independent surface states while the others are field-dependent. We have found a scaling result from which the number of magnetic field-dependent states of large dots can be inferred from those of smaller dots.

PACS numbers:

I. INTRODUCTION

Graphene dots have a great potential for many applications since they are the elemental blocks to construct graphene-based nano devices. It is possible to cut graphene sheet$^1$ in the desired shape and size$^2$, and use it to make quantum dot devices. In such devices it may be possible to realize experimentally zigzag or armchair boundaries.

Graphene systems possess several unusual physical properties associated with the presence of the Dirac points. For example, compared to ordinary Landau levels of quasi-two-dimensional semiconductors the lowest Landau level (LLL) of graphene is peculiar since it has zero energy that is independent of magnetic field$^3$$^7$. Moreover, wavefunctions of the LLL are chiral, i.e., the probability amplitude of find the electron on one type carbon atoms is zero. There are other graphene systems with zero energy states. Semi-infinite$^8$ or nanoribbon graphene$^9$$^{10}$ with zigzag edges along the x-axis develop a flat band of zero energy chiral states. These states are surface states and are localized states at the zigzag edges with various localization lengths$^8$. The zigzag edge and the LLL states have zero energy because their wavefunctions are chiral. Effects of a magnetic field on graphene Hall bars have been investigated recently, and some zero energy chiral states are found to be strongly localized on the zigzag edges in addition to the usual LLL states$^{11}$$^{14}$.

One may expect that the degeneracy of chiral states with zero energy will be split when quantum confinement effect is introduced in a graphene dot$^{15}$$^{17}$. However, the splitting of these energies may be unusual in some graphene dots$^{18}$$^{21}$. Recently the magnetic field dependence of these levels in a gated graphene dot was investigated experimentally$^{21}$. Effects of various types of edges have been also investigated: zigzag-edged dots, armchair-edged dots$^{19}$$^{22}$$^{24}$, and rectangular graphene dots with two zigzag and two armchair edges$^{25}$$^{26}$ have been studied. Armchair edges couple states near K and K’ points of the first Brillouin zone and generate several mixed chiral zigzag edge states with nearly zero energies. In the rectangular dots the number of these states, $N_l$, may be determined from the condition that the x-component of wavevectors satisfies $1/L_y < k_{x,n} < \pi/3a$, where $k_{x,n} = \frac{x}{a} - \frac{n}{3}$, $a = \sqrt{3}a_0$ is the length of the unit cell, and $n = 0, \pm 1, \pm 2, \ldots$ (the nearest neighbor carbon-carbon distance is $a_0 = 1.42\AA$), the horizontal length of the dot is $L_x = \sqrt{3}M a_0$ with $M$ number of hexagons along the x-axis, and the vertical length is $L_y = a_0(3N^2+2)$ with $N$ the number of hexagons and $(N+1)$ carbon bonds along the y-axis. See Fig.1. This condition implies that the integer $n$ is given by

$$\frac{\sqrt{3}M}{(3N+2)\pi} + \frac{2M}{3} \leq n \leq M. \quad (1)$$

The effective mass approximation wavefunctions of these surface states are derived in Ref.$^{20}$.

We investigate how properties of rectangular dots
change in the presence of a magnetic field in the regime where Hofstadter-butterfly effects [18,19,21] are negligible. In neutral graphene dots the Fermi level has zero energy, and, consequently, magnetic, optical, and STM properties are expected to depend on the number of available states near zero energy. Our investigation shows that the wavefunctions of nearly zero energy states are all peaked on the zigzag edges with or without appreciable weight inside the dot. This may be understood as mixing of LLL and surface states by armchair edges of the square dot through intervalley scattering, which is unique to the square dot (This will be explained in Sec.IV).

Our study shows that the number of states within the energy interval $\delta$ around zero energy is given by

$$N_T(\delta) = N_I + N_D(\delta)$$

(2)

(the energy $\delta$ is typically less than the quantization energy of a rectangular dot, which can be estimated using the Dirac equation: $\gamma k_{min} \sim (T_{x,y})$, with $\gamma = \sqrt{3}a/2$ with the hopping energy $t$). Here magnetic edge states are not included since their energies are larger than $\delta$. $N_D(\delta)$ is the number states at zero magnetic field that merge into the energy interval $\delta$ around zero energy as the dimensionless magnetic flux $\phi = \ell / a^2$ increases. This effect provides a means to control the number of states at the Fermi level. There are other states with nearly zero energies at $\phi = 0$, which remain so even at $\phi \neq 0$. The localization lengths of these states are shorter than the magnetic length. We denote the number of these states by $N_I$.

Our numerical results indicate that for relatively small rectangular-shaped graphene dots with size less than or order $10^2 a^2$ the number of states at the Fermi level display a negligible magnetic field dependence for values that are usually accessible experimentally ($B < 10^7$) corresponds, in dimensionless magnetic flux, to $\phi = \Phi_0 / 2 < 10^{-4}$, where $\Phi_0 = h c / e$ and $\Phi = B a^2 / h$, with the area of a hexagon $A_h = 3\sqrt{3}a^2$. On the other hand, in larger dots this dependence is significant. However, it is computationally difficult to investigate large rectangular-shaped graphene dots since the number of carbon atoms increases rapidly with the size. We have found a scaling result from which one can infer results for larger dots from those of smaller dots. For different rectangular-shaped graphene dots and values of $\phi$ it can be described well by the following dimensionless form

$$N_D(\phi) = \frac{L_x L_y}{A_h} f\left(\frac{\ell^2}{\Phi_0 (L_x + L_y)}\right),$$

(3)

where $\ell = \frac{a^2}{\sqrt{3}\Phi_0}$ is the magnetic length and $f(x)$ is a scaling function, see Fig 2. The total number of hexagons in the dot is $N_h = L_x L_y / A_h$. Our numerical result shows that the dependence of $N_D(\phi)$ on $\phi$ is initially non-linear in the regime where the diameter of the cyclotron motion is comparable to the system length, $2\ell \sim L_{x,y}$.

II. NUMBER OF STATES IN THE QUASI-DEGENERATE LEVEL

Our Hamiltonian is

$$H = -\sum_{i,j} t_{ij} c^+_i c_j,$$

(4)

where $t_{ij} = t e^{i \vec{k}_{ij} \cdot \vec{A} d\vec{r}}$ are the hopping parameters and $c_i^+$ creates an electron at site $i$. Here we use a Landau gauge $\vec{A} = B(-y, 0, 0)$. The summation over $i,j>$ is over nearest neighbor sites and $t = 2.5 eV$. The eigenstate with eigenenergy $\epsilon_n$ is denoted by $\phi_{\epsilon_n}(\vec{R})$, where $\vec{R}$ labels each lattice point. Because of electron-hole symmetry eigenvalues appear in pairs of positive and negative values ($\epsilon, -\epsilon$), and the probability wavefunctions of a pair of states, $(|\phi_{\epsilon_n}(\vec{R})|^2, |\phi_{-\epsilon_n}(\vec{R})|^2)$, are identical. Our numerical results are consistent with this.

Figs 3(a) and (b) display the energy spectra near zero energy for $\phi = 0$ and 0.01. At $\phi = 0$ there are approximately 20 states within $|\epsilon| < 0.01 eV$, consistent with the analytical result of Eq. (1). At $\phi = 0.01$ the numerical value is increased to 24. Fig 4(a) shows how some energy levels $\epsilon_n$ at $\phi = 0$ change as a function of the magnetic flux $\phi$. These energy levels do not anticross. We observe that nearly zero energies at $\phi = 0$ do not change noticeably in magnitude as $\phi$ varies. There are $N_I$ such localized surface states. On the other hand, we find that as $\phi$ increases non-zero energies become smaller and move closer to zero. This implies that, for a given energy interval $\delta$, the number of states in it, $N_T(\phi)$, increases with $\phi$. From Fig 3(b) we see that it displays a non-linear dependence on $\phi$. For a large dot of size $50 \times 50 nm^2$ a similar dependence of $N_T$ on $B$ is seen, as shown in Fig 5. Non-linear dependence occurs in the regime $2\ell / L_x \sim 0.5$. As a test of our numerical procedures we have verified that the sum of $N_D(\phi) = N_T(\phi) - N_I$ and the number of magnetic edge states is equal to the total bulk Landau level degeneracy $2D_B (D_B = \frac{2L_x L_y}{3\sqrt{3}\Phi_0})$ is the degeneracy per valley.)
FIG. 3: (a) Eigenenergies $\epsilon_n$ at $\phi = 0$. Quasi-degenerate states are present near zero energy. Size of the dot is $74 \times 71 \text{Å}^2$. A quantization energy of order $\gamma k_{\text{min}} \sim 0.03\text{eV}$ can be seen as an excitation gap near zero energy. (b) Eigenenergies $\epsilon_n$ at $\phi = 0.01$. SIZE OF THE DOT IS $74 \times 71 \text{Å}^2$.

The ratio between the number of nearly zero energy states induced by the magnetic field and the number of hexagons, $\frac{N_D(\phi)}{N_h}$, should depend on a dimensionless quantity consisting of a combination of $\ell$, $a_0$, $L_x$ and $L_y$, which are the important parameters of rectangular graphene dots. The lengths $L_x$ and $L_y$ should appear as $L_x + L_y$ so that for rectangular-shaped graphene sheets $N_D/N_h$ remains the same when $L_x$ and $L_y$ are exchanged. These considerations lead us to the dimensionless variable $\frac{\ell^2}{a_0(L_x+L_y)} = \frac{3}{4\pi} \frac{1}{(M+\sqrt{3}N+2)/\sqrt{3}}$, see Eq. (3).

We are especially interested in the regime where the diameter of the cyclotron orbit is comparable to the system length $2\ell \sim L_{x,y}$. Note that in this regime many cyclotron orbits get affected by the presence of the edges and corners of the rectangular dot. Since we must also assume that Hofstadter effect is negligible the validity regime of Eq. (3) is $a_0 \ll 2\ell < L_{x,y}$. Note also that the scaling function $f(x)$ should be different for each $\delta$.

III. WAVEFUNCTIONS OF QUASI-DEGENERATE STATES IN A MAGNETIC FIELD

We first show how the wavefunction of a non-zero energy state at $\phi = 0$ changes into a state with nearly zero energy as $\phi$ increases. Consider the probability wavefunction for $n = 1027$ at $\phi = 0.01$.
FIG. 7: Size of the dot is 74 × 71 Å². (a) The probability wavefunction of the state with $\epsilon_{1045} = 5.38 \times 10^{-6}$eV at $\phi = 0$. (b) Profile of z-component of pseudospin for $n = 1045$ at $\phi = 0$. (c) The probability wavefunction for $n = 1045$ at $\ell/L_x = 0.12$ ($\phi = 0.01$). (d) Profile of z-component of pseudospin for $n = 1045$ at $\phi = 0.01$.

FIG. 8: Size of the dot is 74 × 71 Å² and $\ell/L_x = 0.09$ ($\phi = 0.02$). (a) The probability wavefunction of the state with $\epsilon_{1027} = -2.04 \times 10^{-5}$eV. (b) Profile of z-component of pseudospin of the same state. These results should compared with those in Fig. 6.

FIG. 9: (a) The probability wavefunction of the state with $\epsilon_{1053} = 0.144$eV at $\ell/L_x = 0.12$ ($\phi = 0.01$). Size of the dot is 74 × 71 Å². (b) Profile of z-component of pseudospin of the same state.

It is localized on the zigzag edges with a finite probability inside the dot. On the armchair edges the wavefunction is vanishingly small. The wavefunction has changed significantly from the $\phi = 0$ result, see Fig. 6(a), and also its energy has changed from $- 0.07$eV to $-2.0 \times 10^{-3}$eV. The values of the z-component of the pseudospin, Fig. 6(b) and Fig. 6(d), are larger on the zigzag edges at $\phi = 0.01$ compared to the result at $\phi = 0$. The probability wavefunction of another state with nearly zero energy is shown in Fig. 7(c) at $\phi = 0.01$. We see that the result is somewhat different from the zero field result of Fig. 7(a), which displays a localized state with the localization length comparable to the unit cell length $a$. Now there is a finite probability to find an electron inside the dot while the probabilities on the zigzag edges are reduced. Note that the energy of this state has changed from $5.38 \times 10^{-6}$eV to $4.5 \times 10^{-6}$eV when $\phi$ is changed to $0.01$ from zero. The pseudospin profiles are shown in Figs. 7(b) and (d). Fig. 8 shows a probability wavefunction at a smaller value of $\ell/L_{x,y} = 0.09$ (corresponding to $\phi = 0.02$), and we see that the wavefunction is less localized on the zigzag edges and LLL character is more pronounced in comparison to result of $\ell/L_x = 0.12$ (Fig. 6(c)). All $N_D(\phi)$ states have similar properties mentioned above with finite probabilities of finding an electron inside the dot. There are also $N_{\ell}$ zigzag edges states that are more strongly localized on the edges with localization lengths comparable to $a$. When an electron is in one of these states the probability of find the electron away from the edges is practically zero. The energies of these states are less then $10^{-10}$eV. We can summarize our results as follows: all nearly zero energy states are localized on the zigzag edges with or without some weight inside the dot.

When the magnetic length is much smaller than the system size magnetic edge states can be formed, see Fig. 9. The probability wavefunction of a magnetic edge state with $\epsilon_{1053} = 0.144$eV is shown in Fig. 9(a). It is a mixture of ordinary magnetic and zigzag edge states. The probability wavefunction decays from the armchair edges while it is strongly peaked on the zigzag edges. Pseudospin expectation values on each zigzag edge display opposite chiral behavior. On armchair edges the chiralities are more or less evenly mixed, see Fig. 9(b).

IV. DISCUSSIONS AND CONCLUSIONS

We now explain qualitatively how mixed states of Fig. 6(c) and Fig. 7(c) can arise. An infinitely long zigzag nanoribbon in a magnetic field has nearly zero energy surface states that are localized on the edges in addition to ordinary lowest Landau level states, see
should display a significant occupation of both A and B in Fig.6(c) and Fig.7(c). In addition, these mixed states weight on the zigzag edges and inside the dot, as shown be coupled and give rise to mixed states with significant consequently, surface and LLL states of a nanoribbon can chair edges couple K and K' of order the carbon-carbon distance various localization lengths but the minimum value is characterized between A and B. The surface states can have of B (A) type and localized surface states have a mixed gauge is used). nanoribbon with infinitely long zigzag edges along the x-axis FIG. 10: Cross section of probability wavefunctions of a | of order the carbon-carbon distance. The armchair edges couple K and K' valleys, and, consequently, surface and LLL states of a nanoribbon can be coupled and give rise to mixed states with significant weight on the zigzag edges and inside the dot, as shown in Fig(c) and Fig(c). In addition, these mixed states should display a significant occupation of both A and B carbon atoms inside the dot since LLL states of different chiralities are coupled by the armchair edges. Our numerical result is indeed consistent with this expectation, see Fig(d). As the ratio $\ell/L_{x,y}$ takes smaller values the nature of these states become more like that of LLL states (see Fig). We have investigated, in the presence of a magnetic field, quasi-degenerate states of rectangular-shaped graphene dots near the Dirac points. Some of these states are magnetic field independent surface states while the other states are field dependent. We find numerically that the wavefunctions of these states are all peaked near the zigzag edges with or without significant weight inside the dot. The physical origin of the presence of a significant weight is the coupling between K and K' valleys due to the armchair edges. This effect is expected to survive small deviations from perfect armchair edges as long as they provide coupling between different valleys. Experimentally the dependence of $N_D$ on $\phi$ may be studied by measuring STM properties or the optical absorption spectrum as a function of magnetic field. In fabricating rectangular dots a special attention should be given to the direction of armchair edges since the properties of dot may depend on it.

Acknowledgments

This work was supported by the Korea Research Foundation Grant funded by the Korean Government (KRF-2009-0074470). In addition this work was supported by the Second Brain Korea 21 Project.

[1] For recent reviews see: T. Ando, J. Phys. Soc. Jpn. 74, 777 (2005); A. K. Geim and A. H. MacDonald, Phys. Today 60 35 (2007); A. H. Castro Neto, F. Guinea, N. M. R. Peres, K. S. Novoselov, and A. K. Geim, Rev. Mod. Phys. 81, 109 (2009).
[2] K. S. Novoselov, A. K. Geim, S. V. Morozov, D. Jiang, Y. Zhang, S. V. Dubonos, I. V. Grigorieva, and A. A. Firsov, Science 306, 666 (2004); H. Hiura, Appl. Surf. Sci. 222, 374(2004); A. K. Geim and K. S. Novoselov, Nat. Mater. 6, 183 (2007).
[3] Y. Zhang, Y.W. Tan, H.L. Stormer, and P. Kim, Nature (London) 438, 201 (2005).
[4] K. S. Novoselov, A.K. Geim, S.V. Morozov, D. Jiang, M.I. Katsnelson, I.V. Grigorieva, S.V. Dubonos, and A.A. Firsov, Nature (London) 438, 197 (2005).
[5] J.W. McClure, Phys. Rev. 104, 666 (1956).
[6] Y. Zheng and T. Ando, Phys. Rev. B 65, 245420 (2002).
[7] S. G. Sharapov, V. P. Gusynin, and H. Beck, Phys. Rev. B 69, 075104 (2004).
[8] M. Fujita, K. Wakabayashi, K. Nakada, and K. Kusakabe, J. Phys. Soc. Jpn. 65 ,1920 (1996).
[9] L. Brey and H. A. Fertig, Phys. Rev. B 73, 195408 (2006).
[10] Y. W. Son, M. L. Cohen, and S. G. Louie, Phys.Rev.Lett. 97, 216803 (2006).
[11] L. Brey and H. A. Fertig, Phys. Rev. B 73, 235411 (2006).
[12] A. H. Castro Neto, F. Guinea, and N. M. R. Peres, Phys. Rev. B 73, 205408 (2006).
[13] V. P. Gusynin, V. A. Miransky, S. G. Sharapov, I. A. Shovkovy and C. M. Wyenberg, Phys. Rev. B 79, 115431 (2009).
[14] M. Arikawa, Y. Hatsugai, and H. Aoki, Phys. Rev. B 78, 205401 (2008).
[15] A. DeMartino, L. Dell’Anna, and R. Egger, Phys. Rev. Lett. 98, 066802 (2007).
[16] G. Giavaras, P. A. Maksym, and M. Roy, J. Phys.: Condens. Matter 21, 102201 (2009).
[17] W. Häusler, and R. Egger, arXiv:0905.3667v1.
[18] S. Schnez, K. Ensslin, M. Sigrist, and T. Ihn, Phys. Rev. B 78, 195427 (2008).
[19] Z. Z. Zhang, K. Chang, and F. M. Peeters, Phys. Rev. B 77, 235411 (2008).
[20] P. Recher, J. Nilsson, G. Burkard, and B. Trauzettel, Phys. Rev. B 79, 085407 (2009).
[21] J. Güttinger, C. Stampfer, F. Libisch, T. Frey, J. Burgdörfer, T.Ihn, and K. Ensslin, cond-mat arXiv: 0904.3506v2.
[22] J. Fernández-Rossier and J. J. Palacios, Phys. Rev. Lett. 99, 177204 (2007).
[23] M. Ezawa, Phys. Rev. B 76, 245415 (2007).
[24] O. Hod, V. Barone, and G. E. Scuseria, Phys. Rev. B 77, 035411 (2008).
[25] B. Trauzettel, D. V. Bulaev, D. Loss and G. Burkard,
Nature Phys. 3, 192 (2007).
[26] C. Tang, W. Yan, Y. Zheng, G. Li, and L. Li, Nanotechnology, 19, 435401 (2008).
[27] Y. Niimi, H. Kambara, T. Matsui, D. Yoshioka, and H. Fukuyama, Phys. Rev. Lett. 97, 236804 (2006).
[28] M. O. Goerbig, J. -N. Fuchs, K. Kechedzhi, and V. I. Fal’ko, Phys. Rev. Lett. 99, 087402 (2007).
[29] V. P. Gusynin, S. G. Sharapov, and J. P. Carbotte, Phys. Rev. Lett. 98, 157402 (2007).
[30] H. Hsu and L. E. Reichl, Phys. Rev. B 76, 045418 (2007).
[31] M. Kohmoto and Y. Hasegawa, Phys. Rev. B 76, 205402 (2007).
[32] L.Brey and H.A. Fertig, Phys. Rev. B 75, 125434 (2007).
[33] A. R. Akhmerov and C.W.J. Beenakker, Phys. Rev. B 77, 085423 (2008).