International Journal of Chemical, Materials and Biomolecular Sciences
ISSN: 2415-6620
Vol:10, No:1, 2016

Magnetic Field Effects on Parabolic Graphene Quantum Dots with Topological Defects

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***Abstract*—**In this paper, we investigate the low-lying energy levels of the two-dimensional parabolic graphene quantum dots (GQDs) in the presence of topological defects with long range Coulomb impurity and subjected to an external uniform magnetic field. The low-lying energy levels of the system are obtained within the framework of the perturbation theory. We theoretically demonstrate that a valley splitting can be controlled by geometrical parameters of the graphene quantum dots and/or by tuning a uniform magnetic field, as well as topological defects. It is found that, for parabolic graphene dots, the valley splitting occurs due to the introduction of spatial confinement. The corresponding splitting is enhanced by the introduction of a uniform magnetic field and it increases by increasing the angle of the cone in subcritical regime.

***Keywords*—**Coulomb impurity, graphene cones, graphene quantum dots, topological defects.

I. Introduction

SINCE the successfully experimental realization [1], [2] of graphene, a new research area [3], [4] developed in the field of condensed matter physics and material science. This material exhibits unusual physical properties, high crystal quality, and exotic Dirac-type spectrum which is described by the analogy with the relativistic Dirac equation [5], [6]. The low-energy dispersion of electrons in graphene is occurred near two unequivalent points in the Brillouin zone: K and K' points [6], where a new pseudospin degree of freedom appears due to the two sublattices defining the honeycomb lattice of graphene. This area has attracted considerable attention by both experimental and theoretical condensed matter physicists due to its novel physical properties. In particular, GQDs have been extensively studied in the recent literature. It has been shown that their controllable various geometries and sizes make them potential candidates for the future electronic and optical devices [7]-[13].

As known, electrons can be described by a two-dimensional Dirac-Weyl equation and behave as massless chiral fermions. Due to this unique property, electrons in graphene cannot be efficiently confined within finite spatial areas and cannot be localized by time like confinement potentials. The confinement of electrons in graphene is not trivial due to the Klein's paradox, which makes potential barriers transparent for normally incident quasi-particles. This problem has been studied in many theoretical investigations by using various confinement geometries within the different schemes [14]-[36]. Another alternative approach to confine Dirac electrons in graphene have been proposed in the presence of inhomogeneous magnetic fields [16], [25]. In addition, there have been extensive studies on the electronic properties of the topological defects in graphene, i.e., graphene cones [37]-[39]. These structures can be realized by distortions of graphene sheets by introducing various kinds of defects. These defects induce lattice distortions that can be generally classified in two types of dislocations and disclinations. Dislocations type disorders arise from the translational lattice incompatibility of the crystal lattice. In the presence of dislocations, an extra vector has to be introduced, which is called the Burgers vector [40]-[42]. Disclinations are defects that are originating from the rotational incompatibility of the crystal lattice, and these are equivalent to wedge disclinations. Disclination on a 2D graphene can be thought of an explicit breaking of the local rotational symmetry which can be measured by the Frank's vector [41].

The purpose of this work is twofold: First, we examine the electronic properties of the parabolic GQDs in the vicinity of the K-point of the Brillouin zone of the gapped graphene by using the effective low-energy Dirac equation for the electron quasi-particle states in the presence of a single charged Coulomb impurity that is subjected to a homogeneous magnetic field. The second one includes the physics of graphene cones. In this paper, we examined the electronic properties of parabolic QDs with topologically defected graphene i.e. graphene cone. The energy levels of GQD in the presence of defects and subjected to a uniform magnetic field perpendicular to GQD plane are studied in this context within the framework of the perturbation theory.

The paper is organized according to the following order: In Section II, first, the model is introduced and following the introduction the electronic properties of parabolic GQDs is described and discussed. In Section III a brief summary and conclusion is added.

II. Theory

Electrons near the K-point of the graphene obey the massless relativistic Dirac equation. The effective Hamiltonian in the presence of a constant uniform magnetic field and a parabolic confinement potential with a single charged Coulomb impurity is given by

$$H = v_F \vec{\sigma} \cdot \left(\vec{p} + \frac{e}{c}\vec{A}\right) - \frac{Ze^2}{\epsilon r} + \tau\, m v_F^2 \sigma_z + \beta \Delta r^2 \,. \qquad (1)$$

σ_i and β are Dirac matrices, $v_F = (3a/2)J_0$ is the Fermi velocity and J_0 is the resonance integral between nearest neighbor carbon atoms which is of order of 2.7 eV. Here, a is

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the equilibrium bond length of the graphene. $\vec{p} = -i\hbar\vec{\nabla} = -i\hbar(\partial_x, \partial_y)$ is the two-dimensional momentum operator, $\boldsymbol{A}$ is the vector potential that generates the magnetic field $\boldsymbol{B} = \boldsymbol{\nabla} \times \boldsymbol{A}$, and it will be chosen in the symmetric gauge, i.e., $\boldsymbol{A} = \mathrm{B}(-\mathrm{y}, \mathrm{x}, 0)/2$, and Ze^2/ϵ is the strength of a charged impurity, where Z is the atomic number of impurity, ϵ is the dielectric constant. The third term in (1), is the mass term and it gives rise to an energy gap $2mv_F^2$ in the spectrum of graphene, where $\tau = +1$ ($\tau = -1$) corresponds to the K (K') valley. Throughout this work, we restrict ourselves to a single valley (K) and a single band (conduction). The last term in (1) corresponds to GQD potential wherein $\Delta = U_0/2R_0^2$, U_0 and R_0 are the strength and the radius of the graphene quantum dot, respectively. The solution of (1) in the absence of parabolic potential is well established in [39] in terms of spinor wave function, $\Psi_{A,B}^{\dagger} = \left(\Psi_{AB+}^{\dagger}\ \Psi_{AB-}^{\dagger}\right)$ where A and B are the pseudospin indices and refer to sublattices of graphene, while $+$ and $-$ signs denote the valleys.

In order to get conical topology or topological defects in graphene, one needs to introduce nontrivial holonomies in the pseudoparticle wave function. In the presence of a graphene cone with an angle of deficit $2\,n_\Omega\pi/6$, the angular boundary condition on spinor wave function Ψ is given by

$$\Psi(r, \theta = 2\pi) = e^{ie2\pi r\left(1-\frac{n_\Omega}{6}\right)}\Psi(r, \theta) \tag{2}$$

where n_Ω is defect number of topological defects. These holonomies on spinor wave function can be represented by a fictitious gauge field here n_Ω is defect number of topological defects, and these holonomies on spinor wave function can be formed with fictitious gauge field

$$A_\theta(r) = \frac{1}{er}\left[\pm\frac{n_\Omega/4}{1-n_\Omega/6}\sigma_0 + \frac{1}{2}\sigma_3\right] \tag{3}$$

By inserting this fictitious gauge field into (1), the effective Hamiltonian for the low-energy excitations of a graphene cone in the presence of both parabolic QD and a single charged Coulomb impurity subjected to a homogeneous magnetic field can be written as a sum of three Hamiltonians, $\bar{H} = H_0 + H' + H''$ in units of $\hbar v_F$:

$$H_0 = \begin{pmatrix} m_0 - \frac{\bar{Z}}{r} & \frac{\partial}{\partial r} - \frac{i}{r\left(1-\frac{n}{6}\right)}\frac{\partial}{\partial\theta} \pm \frac{n/4}{r\left(1-\frac{n}{6}\right)} + \frac{1}{2r} \\ -\frac{\partial}{\partial r} - \frac{i}{r\left(1-\frac{n}{6}\right)}\frac{\partial}{\partial\theta} \pm \frac{\frac{n}{4}}{r\left(1-\frac{n}{6}\right)} - \frac{1}{2r} & -m_0 - \frac{\bar{Z}}{r} \end{pmatrix} \tag{4}$$

together with

$$H' + H'' = \begin{pmatrix} \Delta_0 r^2 & \bar{B}r/2a^2 \\ -\bar{B}r/2a^2 & -\Delta_0 r^2 \end{pmatrix}. \tag{5}$$

In (5), $\bar{B} = B/B_0$ is the dimensionless magnetic field, $B_0 = \hbar c/ea^2$, and $\bar{Z} = Ze^2/\epsilon\hbar v_F$ is the dimensionless coupling constant. Here, we have also used the abbreviations $m_0 = mv_F/\hbar$ and $\Delta_0 = \Delta/\hbar v_F$. H_0 is the exactly solvable and its corresponding energy eigenvalues are found to be

$$\bar{\varepsilon}_n = m_0\left[1 + \bar{Z}^2/\left(n + \sqrt{\nu^2 - \bar{Z}^2}\right)^2\right]^{-1/2} \tag{6}$$

together with the corresponding eigenfunctions in terms of Laguerre polynomials

$$\Psi_{n,j}(r) = \begin{pmatrix} F_{nj}(r)e^{i\theta(j-1)} \\ iG_{nj}(r)e^{i\theta(j)} \end{pmatrix} \tag{7}$$

where

$$\left.\begin{matrix}\mathrm{F_{nj}(r)} \\ \mathrm{G_{nj}(r)}\end{matrix}\right\} = \begin{matrix}(-1)^n N_{n,j}(m_0, \bar{Z})\sqrt{m_0 \pm \varepsilon_0}\ e^{-\lambda r} \\ \times (2\lambda r)^{\gamma-1/2}\left[L_n^{2\gamma}(2\lambda r) \pm C_{21}L_{n-1}^{2\gamma}(2\lambda r)\right]\end{matrix}$$

with a normalization constant

$$N_{n,j}(m_0, \bar{Z}) = \left\{\frac{\Gamma(n+1)\lambda^3\left[j + \sqrt{\bar{Z}^2 + (n+\gamma)^2}\right]}{\Gamma(n+2\gamma+1)\ {m_0}^2\bar{Z}}\right\}^{1/2}$$

and here $C_{21} = -(n+2\gamma)/(j + m_0\bar{Z}/\lambda)$, where $\lambda = m_0\bar{Z}/\sqrt{\bar{Z}^2 + (n+\gamma)^2}$, $\gamma = \sqrt{\nu^2 - \bar{Z}^2}$ with $\nu = (j \pm n_\Omega/4)/(1 - n_\Omega/6)$ which depends on j as well as the number of sectors n_Ω removed from the gapped graphene to from conical topological defects. $j = m_j + 1/2$ is the eigenvalue of the conserved total angular momentum J_z. The quantum number n takes values $n = 0,1,2,\ldots$ if $m_j \geq 0$, and $n = 1,2,\ldots$ if $m_j < 0$. It can be easily checked that the lowest angular momentum channel is $j = \pm 1/2$, the critical coupling constant $\bar{Z}_c$ takes the well-known value, i.e., 0.5 for the case $n = 0$, and it increases by increasing the angle of the cone, except for the case of $n_\Omega = 2$. In our calculations, we have excluded the $n_\Omega = 2$ case, because it is required that supercritical regime. In the framework of perturbation theory, by using corresponding eigenfunctions and obtained the first-order shift in energy eigenvalues of (1) as $\bar{E} = \bar{\varepsilon}_n + \Delta\bar{\varepsilon}_n{}' + \Delta\bar{\varepsilon}_n{}''$, where

$$\Delta\bar{\varepsilon}_n{}' = \begin{matrix}\left(\bar{B}/4\bar{m}_0[\bar{Z}^2 + (n+\gamma)^2]^{\frac{1}{2}}\right) \\ \times\left[\left(2n + \sqrt{\nu^2 - \bar{Z}^2}\right)\nu + (\bar{Z}^2 + (n+\gamma)^2)^{1/2}\right]\end{matrix} \tag{8}$$

is the Zeeman term due to magnetic field and this result is valid for $\bar{B} \ll \bar{Z}^2\bar{m}_0{}^2/2$ and

$$\Delta\bar{\varepsilon}_n{}'' = \left(1/4\bar{R}^3\bar{Z}\bar{m}_0{}^2\sqrt{\bar{m}_0{}^2 - \bar{\varepsilon}_n{}^2}\right)[2\,\bar{m}_0 n(n+\gamma)(n+2\gamma) + \bar{\varepsilon}_n\bar{Z}\,\bar{m}_0/\sqrt{\bar{m}_0{}^2 - \bar{\varepsilon}_n{}^2}\,[2(n+\gamma)^2 + n(n+2\gamma)+1] + 3\bar{\varepsilon}_n(n+\gamma)\nu] \tag{9}$$

is the contribution due to parabolic quantum dot potential. Thus, the energy eigenvalues can be written as,

$$\bar{E} = m_0\left[1+\bar{Z}^2/\left(n+\sqrt{\nu^2-\bar{Z}^2}\right)^2\right]^{-1/2} + \left(\bar{B}/4\bar{m}_0[\bar{Z}^2+(n+\gamma)^2]^{\frac{1}{2}}\right)[\left(2n+\sqrt{\nu^2-\bar{Z}^2}\right)\nu + (\bar{Z}^2+(n+\gamma)^2)^{\frac{1}{2}}] + \left(1/4\bar{R}^3\bar{Z}\bar{m}_0{}^2\sqrt{\bar{m}_0{}^2-\bar{\varepsilon}_n{}^2}\right)[2\,\bar{m}_0 n(n+\gamma)(n+2\gamma) + \bar{\varepsilon}_n\bar{Z}\,\bar{m}_0/\sqrt{\bar{m}_0{}^2-\bar{\varepsilon}_n{}^2}\,[2(n+\gamma)^2 + n(n+2\gamma)+1] + 3\bar{\varepsilon}_n(n+\gamma)\nu] \quad . \quad (10)$$

Due to the parabolic confinement effect, the energy of topologically defected graphene cone is increased by increasing the dot radius. Indeed, in Fig. 1, for the constant effective dot strength $U_0 = 0.4\ meV/nm^2$, we have plotted the kinetic energies given by (10) for two $n_\Omega = 0$ and $n_\Omega = 1$, respectively, in the presence of four different strength magnetic fields. For, $n_\Omega = 0$ (straight lines), we have lowered energy levels as compared to the $n_\Omega = 1$ (dashed lines) case. When the magnetic field tends to the higher values, Landau levels of the gapped structure are restored in the presence of pentagonal defect at the apex of the cone. In order to better understand how the magnitude of these level splittings change with magnetic field and dot strength, we have provided also plots in Fig. 2, for the second low-lying state, i.e., $n = 1$ and for the first angular momentum channel $j = 1/2$, in the presence of triangular defect in the apex of the cone. In this figure, straight lines represent the $1\ Mev/nm^2$ dot strength; dashed lines show the $0.5\ Mev/nm^2$ dot strength. In this figure, it should be noted that the level spacing is sensitive to the changes in the parabolic dot strength. Additionally, the difference of energy levels decreases by increasing dot radius.

In order to understand the influence of combined effects of potentials, we have also plotted eigenenergies as a function of dot radius $R = (\hbar v_F R_0^2/U_0)^{1/3}$ for a constant magnetic field, $B = 5\,T$ in Fig. 3. As can be seen from this figure, energy values in the presence of parabolic confinement potential becomes weaker by the increase of dot radius. We also give the corresponding energy dependences in Fig. 3, both for various topological defects, and various parabolic dot potential strengths.

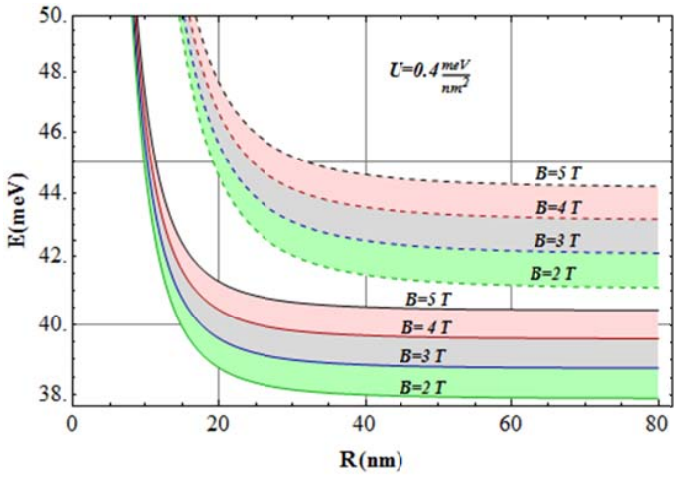

Fig. 1 The energy levels obtained for $n_\Omega = 0$(graphene sheet) and $n_\Omega = 1$ (pentagonal defect at the apex of the cone) in the presence of different magnetic field values

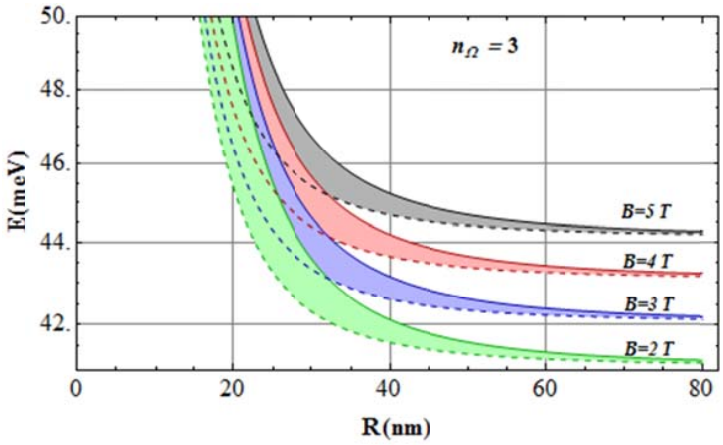

Fig. 2 The lowest-lying energy levels of parabolic GOD as a function of quantum dot radius $R = \left(\hbar v_F {R_0}^2/U_0\right)^{1/3}$ in the presence of a triangular defect at the apex of the cone

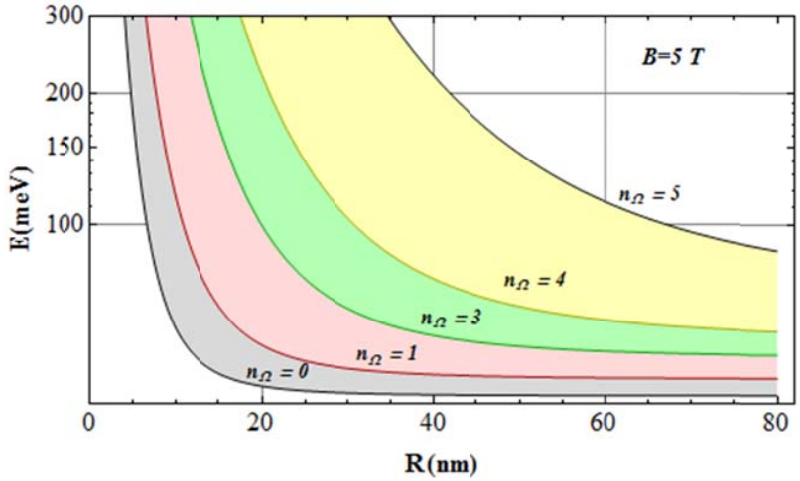

Fig. 3 The energy levels is plotted as a function of dot strength. In the presence of the different topological defects, i.e., graphene cones, with a charged Coulomb impurity

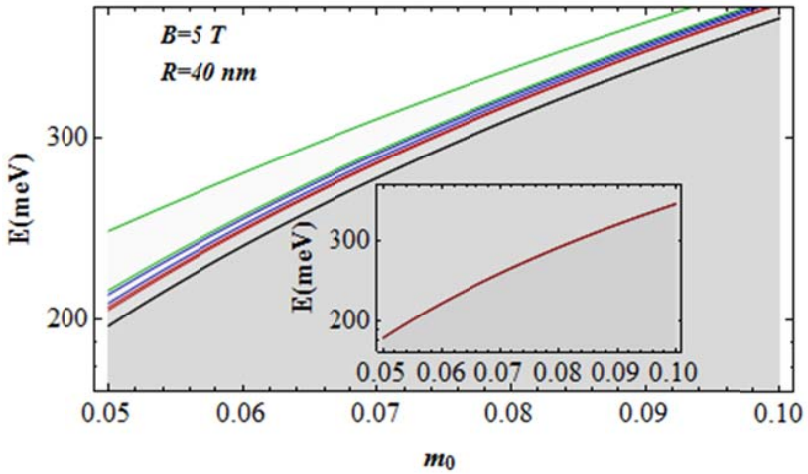

Fig. 4 Pseudo-Zeeman splitting due to topological defects as a function of the gap parameter, m_o is plotted for fixed values of magnetic field and dot radius, $B = 10\,T$ and $R = 40\,nm$. Inset: In the absence of topological defects energy values are degenerate

From Fig. 4 it can be seen that, increasing the mass gap term also enhances the level spacing. The level spacing strongly depends on the number of sectors removed from the gapped graphene to form topological defects.

For $n_\Omega = 0$ (inset in Fig. 4) even in the presence of the magnetic field $B = 10\,Tesla$, with dot potential or without potential situation have no difference from each other. However, in case topological defects are injected in graphene, these two situations differentiate from each other on the condition that we analyze as a function of mass parameter. We also show that, by the increase of mass parameter, energy levels increase as well. We have found that the highest contribution to the energy eigenvalues comes from the pentagonal defect and small values of dot radius.

III. Conclusion

In summary, we have presented a calculation of energy levels of GQD in the presence of topological defects with long range Coulomb impurity which is subjected to an external uniform magnetic field. The energy difference occurs due to the presence of a spatial confinement potential and it continues to increase as the radius decreases. Consequently, we have shown how to control the energy levels by geometrical parameters of a quantum dot with topological defects and by the strength of uniform magnetic field. The possibility of controlling their physical parameters such as their shapes and sizes makes these system ideally suited for the investigation of the electronic properties of this system. We think that, our results will provide a deep understanding for the electronic properties of graphene and graphene cones.

Acknowledgment

This work was supported by TUBITAK under Grant no.113F103.

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