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The Effect of Tilted Magnetic Field in Graphene Cone

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Abstract

We investigate the combined effect of both homogeneous and tilted magnetic fields on the energy spectrum of gapped graphene cones together with long range Coulomb impurity in the framework of perturbation theory. The results illustrate that the tilted magnetic field can significantly affect the spectrum of single particle low-energy effective Hamiltonian, besides lifting the degeneracy of angular momentum channels in the presence of topological defects. The breaking of the electron-hole symmetry by magnetic fields is explained as a direct consequence of sub band Landau-level coupling.

Keywords: Graphene cones, Tilted magnetic field, Topological defects

1. Introduction

Since the discovery of graphene, there has been a growing interest in studying the physical properties of graphene and graphene-based microstructures since their experimental realization (Novoselov et. al., 2004; Wallace, 1946). Graphene and structurally similar materials show an amazing versatility to form a wide variety of unusual morphologies. This variety of morphologies results from distortions of graphene sheets by the incorporation of various defects such as dislocations and disclinations. Dislocations are crystal defects arising from translational lattice incompatibility, as measured by the Burgers vector (Bakke & Furtado, 2013; Juan, Cortijo, & Vozmedia, 2010; Kochetov, Osipov, & Pincak, 2010), whereas disclinations are defects originating in the rotational incompatibility of the crystal lattice, as characterized by the Frank's vector(Kochetov, Osipov, & Pincak, 2010). We interested in disclinations. Disorder plays a very important role in the electronic properties of low-dimensional
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In particular, recent researches have shown that the topological defects, which are inherent to its own geometry (Pachos, 2009; Neto et. al, 2009; Furtado et. al, 2008), has generated considerable interest. Also, the effect of various impurities in graphene has been studied extensively (Ostrovsky et. al., 2006; Kastnelson, 2006; Vitor et. al., 2007; Fogler et. al., 2007; Shytov et. al., 2007; Novikov, 2007; Terekhov et. al., 2008; Kotov et. al., 2008; Chen et. al., 2008; Pereira et. al., 2008; Kastnelson & Geim, 2008; Zhu et. al., 2009; Altanhan & Kozal, 2012; Zhu & Sun, 2012).

In this paper, our problem is expressed in two parts, the first is in the vicinity of the K-point of the Brillouin zone of gapped graphene, the effective low-energy Dirac equation for the electron quasi-particle states in the presence of a single charged Coulomb impurity subjected to a homogeneous magnetic field and a tilted magnetic field. The second one is graphene cones (Lambert & Crespi, 2000; Lammert & Crespi, 2004; Cortijo & Vozmedea, 2007; Sitenko & Vlasii, 2007; Yazyev & Louie, 2010; Sun & Zhu, 2014; Liu et. al., 2013; Chakraborty et. al., 2011; Kandemir & Akay, 2015) which are graphene surfaces containing one to five pentagonal defects. These graphenes with topological defects are called graphitic cones. Tunneling electron microscopy, scanning electron microscopy and field emission scanning electron microscopy has provided considerable experimental support for these predicted topological effects (Jaszcak et. al., 2003).

2. Theory

The Hamiltonian of graphene electronic states in the presence of a single charged Coulomb impurity subjected to a homogeneous magnetic field perpendicular to the graphene plane can be defined as,

\[ H_n \psi = \left[ v_F \sigma \left( \frac{p}{\hbar} + \frac{e}{c} A \right) + \sigma_\parallel \left( \frac{e\hbar^2}{2m_e} \right) + \sigma_\parallel m g \mu_B B \right] \psi \]

and corresponding energy eigenfunctions of this Hamiltonian can constructed in terms of pseudospinors

\[ \psi_{\uparrow \uparrow} = \left( \begin{array}{c} \psi_1 \\ \psi_2 \end{array} \right) \]

In a graphene sheet the conduction and valence bands consisting of \( n \) orbitals cross at K and K’ points of the Brillouin zone, where the Fermi level is located. \( \alpha \) and \( \beta \) are pseudospin indices and they refer to the sublattices of graphene. In Eq.(1), \( v_F = 3t_0 a / 2 \approx 10^6 \text{m/s} \) is the Fermi velocity of the electron where \( a \) is the bond length of graphene and \( t_0 \) is the hopping integral. \( \sigma_\parallel \) are Pauli matrices, \( A \) is the vector potential to be chosen in symmetric gauge, \( \mu_B \) is the Bohr magneton. The Dirac fermions result from the honeycomb lattice structure in graphene. Graphene has a planar geometry, but in the presence of a topological defect, the geometry becomes conical. The topological lattice defects in graphene, are equivalent to wedge declinations. Declination on a 2D graphene can be thought of as arising due to an explicit breaking of the local rotational symmetry. This breaking can be enforced by topologically nontrivial external gauge field (Chakraborty et. al., 2011) that carries the declination charge, \( n_{\text{def}} \). In other words, when a graphene cone with an angle of deficit \( 2n_{\text{def}} \pi / \theta_{\text{def}} \) is formed from graphene introducing a topological defect, the angular boundary condition is given by

\[ \psi(r, \theta = 2\pi) = e^{i 2m_\parallel (1 - E_{\text{def}})} \psi(r, 0) \]

So, the all effects of these holonomies on \( \psi \) can be described through nontrivial gauge field \( A_{\parallel}(r) \).
\( A_g(x) = \frac{1}{2\pi} \left[ \frac{H_p}{r_1 - r_0} - \frac{H_n}{r_2 - r_0} \right] \)  

(3)

This topologically induced gauge field inserted into Eq.(1). It is well known that the application of a magnetic field changes drastically the physical properties of the system and its energy spectra.

We know that the tilted magnetic field expression is as (Zheng et.al., 2013),

\[ B = B_1 + B_0 = B(\sin \varphi \cos \theta + \sin \varphi \sin \theta + \cos \varphi) \]

where \( \varphi \) is the tilt angle and \( \theta \) is the azimuthal angle in two-dimensional (2D) plane. The resulting effective Hamiltonian for the low energy excitations of graphene cone with a tilted magnetic field (Georbig et. al., 2008) and magnetic field originated from canonical momentum in the presence of a charged Coulomb impurity placed at the apex can be expressed as a sum of two Hamiltonian

\[ H = H_0 + H' \]

(4)

together with

\[ H' = \begin{pmatrix} 0 & \frac{\delta}{\partial \phi} \left( A_{\phi} + i A_{\phi} \right) + g \mu_B B_0 e^{-i\phi} \\ \frac{\delta}{\partial \phi} \left( A_{\phi} + i A_{\phi} \right) + g \mu_B B_0 e^{-i\phi} & 0 \end{pmatrix} \]

(5)

To constitute tilted magnetic field, we choose the symmetric gauge for the vector potential of vertical magnetic field \( A_1 = B_1 (-y, x, 0)/2 \), is relevant to the electronic canonical momentum and the Landau gauge for the vector potential of in-plane magnetic potential \( A_0 = (2B_2 x, 2B_2 y, 0) \). Eq.(4) can be exactly solvable because the magnetic field term behave like a mass term and corresponding energy eigenvalues are easily found to be

\[ E_n = \frac{g \mu_B B_1 (2n_0 + 1)}{[1 + \alpha^2 / (2 + \sqrt{4\alpha^2})]^2} \]

(6)

together with the corresponding eigen functions in terms of \( F_{n,j} \) and \( G_{n,j} \), Laquerre polynomials

\[ \psi(r, \theta) = \begin{pmatrix} F_{n,j} e^{i\phi} \phi^{-1 - \alpha} \\ G_{n,j} \phi^{1/2} \phi \end{pmatrix} \]

(7)

\[ F_{n,j} = (-1)^n N_{n,j} \left( 2g \mu_B B_0 / \alpha \right) \sqrt{g \mu_B B_0 / \alpha \phi} \times e^{-i\phi} (2\lambda \phi)^{1/2} \left[ L^0_2 (2\lambda \phi) \pm C_{\alpha} L^2_2 (2\lambda \phi) \right] \]

\[ N_{n,j}(g \mu_B B_0 / \alpha) = \left[ \frac{\Gamma(n + 1) \lambda^{1/2} [1 + g \mu_B B_0 / \alpha]}{\Gamma(n + 2\lambda + 1) (g \mu_B B_0 / \alpha)^{1/2}} \right]^{1/2} \]
is the normalization constant, and 

\[ C_{2\ell} = -\frac{\alpha + \beta}{\alpha \ell + \beta \ell + 1 \ell + 1 / 2} \]

with \( \alpha = \left( \sqrt{j(j+1)} \right) / \left( 1 - \frac{\sqrt{j(j+1)}}{\sqrt{j(j+1)}} \right) \), which depends on \( j \) as well as the number of sectors removed from the gapped graphene to form the topological defect. \( j = n_j + 1 / 2 \) is the eigenvalue of the total angular momentum \( J_z \), and the quantum number \( n \) takes values 0, 1, 2, ... if \( m_j \geq 0 \), or it takes values 1, 2, 3, ... for \( m_j < 0 \).

We should note that, for the lowest angular momentum channel \( j = \pm 1 / 2 \) first the critical coupling constant \( \alpha_c \) takes the well known value i.e., 0.5 for the case \( \nu = 0 \), and it increases with increasing the angle of the cone, except for the case of \( n = 2 \) where it is zero. In Eq.(5) the vertical magnetic field components are described by the dimensionless magnetic field as \( \frac{eB}{\hbar c} = B/B_0 = B \), in terms of \( B_0 = 3.10 \times 10^7 \) and \( \alpha = 1.12 \times 10^{-10} \). The effect of the tilted magnetic field on the critical coupling constant for the gapped graphene cone arising from simultaneous effect of \( B_0 \) term of in Eq(4) and term of \( B \) in Eq(5). So, the effects of the tilted magnetic field and the homogeneous magnetic field can be analyzed by use of perturbation theory to determine the first order correction to the energy eigenvalues of Eq(7) as

\[ \Delta E_{n,j} = \int \alpha^2 \varphi^2 \]  

with the result

\[ \Delta E_{n,j} = \frac{1}{4(\text{dim})^2} \frac{\hbar}{\mu_0 B^2} \left\{ \left( 2n + \sqrt{n^2 - j^2} \right) \right\} \left\{ \frac{\hbar}{\text{dim}} \right\} \left\{ \frac{\hbar}{\mu_0 B^2} \right\} \alpha \phi \phi . \]  

(8)

Thus, the energy eigenvalues in the presence of magnetic field can be written as,

\[ \varepsilon_{n,j} = \frac{\hbar}{\text{dim}} \left\{ \frac{\hbar}{\mu_0 B^2} \right\} \alpha \phi \phi \left\{ \left( 2n + \sqrt{n^2 - j^2} \right) \right\} \left\{ \frac{\hbar}{\text{dim}} \right\} \left\{ \frac{\hbar}{\mu_0 B^2} \right\} \alpha \phi \phi . \]  

(9)

In this paper, we present the effect of a tilted and a perpendicular magnetic field on the critical coupling constant for gapped graphene cone arising from sum of Eq.(4) and Eq.(5). So, by employing the perturbation method and only keeping the first order correction of Eq(8), we obtain the eigen values of the system.

To understand how the magnitude of this level splitting changes with a magnetic field originated from canonical momentum, we choose \( B_1 = 0 \) plots in FIG. 1 in the absence of the tilted magnetic field, for the first low lying states, i.e., \( n = 0 \) and for the first two angular momentum channels, i.e., \( j = 1 / 2, 3 / 2 \) and \( j = -1 / 2, -3 / 2 \), respectively in the absence of topological defect \( \nu_j = 0 \) with in the absence of gap parameter (dot-dashed curved), in the absence of topological defect with in the presence of gap parameter (straight line) and in the presence of topological defect \( \nu_j = 1 \), i.e., pentagonal defects on the apex of the graphene with gap parameter(dashed line). It is easily seen that the first energy levels are degenerate with respect to four lowest angular momentum channels, the degeneracy is removed by the introduction of the magnetic fields. Also, from the figures, we compare these three situations, in the presence of topological defect level splitting is further enhance so topological defects behave like a magnetic field and in the presence of gap parameters enhance level splitting and influence the energy spacing.
Fig. 1. The first energy levels \((n = 0, j = \pm 1/2)\), obtained in the absence of the tilted magnetic field for different situations. Dot-dashed curves, in the absence of topological defects and gap parameters; straight lines, in the absence of topological defects and constant gap parameter; dashed lines, have both topological defects (pentagonal defects on the apex of the graphene cone) and constant gap parameter.

The ratio of the parallel magnetic field component of the external magnetic field \(B_p\) to perpendicular magnetic field component of the external magnetic field \(B_L\) gives the tilted magnetic field degree. And we show this degree with \(T_{B} = \frac{H_1}{B_L}\). In FIG.2 the graphic shows the ratio of the parallel magnetic field components for in the presence of the topological defects, and defect number \(n_d = 1\), i.e., pentagonal defects on the apex of the graphene cone for different gap parameter and, perpendicular magnetic field \(B_L = 0.1, 0.2, 0.3\) respectively. Again, the ratio of the parallel magnetic field components to perpendicular magnetic field components for in the absence of topological defects, i.e., for flat graphene for different gap parameter.
From the figures, it is easily seen that the level spacing increases with increasing of the tilted magnetic fields for flat graphene and in the presence of pentagonal defects. Additionally, this level spacing strongly depends also on the defects number of the graphene cone. Moreover, we have analyzed Eq.(9) in FIG.2 in which all assessment of this calculation, we only consider azimuth angle $\varphi = 0$. If we take cognizance of the azimuth angles, it is influence of the tilted magnetic fields degree. Because, the ratio of the parallel magnetic field component of the external magnetic field to perpendicular magnetic field component of external magnetic field is also depend on the azimuth angle like

![Fig. 2](image)

Fig. 2. The ratio of the parallel magnetic field components to perpendicular magnetic field components for in the presence of the topological defects, and defects number $n_{\text{v}} = 1$, i.e., pentagonal defects on the apex of the cone for different gap parameter, i.e., perpendicular magnetic field $B_{\perp} = 0, 0.3, 0.6$ respectively. Inset: The ratio of the parallel magnetic component of the external magnetic field to perpendicular magnetic field component of the external magnetic field is depends also on the azimuth angle like this $T_2 = B_{\parallel}/B_{\perp}$. This can also be justified from the inset which shows how the magnitude of this level splitting changes with azimuth angle.

In FIG.3(a) for $B_{\parallel} = 0.1$ we plot the magnitude of pseudo-Zeeman splitting due to the magnetic field originated from canonical momentum, the first scaled energies given by Eq.(8), for four $n_{\text{v}}$ sectors, $n_{\text{v}} = 1, 2, 3, 4, 5$ (defect conditions), respectively in the tilted magnetic fields $T_{\parallel} = 1$ and $T_{\parallel} = 0.25$. We choose different tilted magnetic field degree to show this enhancement of the level splitting changes with tilted magnetic field degree. Defect number also changes the critical coupling constant. $\alpha_c$ takes the well known value, i.e., $0.5$ for the case $\alpha = 0$, and it increases with increasing the angle of cone, except for the case of $\alpha = 2$ where it is zero so in our calculations we exclude $\alpha = 2$ case. In FIG.3(b), in the constant
tilted magnetic field degree $T_2 = 0.25$ and constant defect number $n_0 = 1$ for the first-two low lying states, i.e., $n = 0$ and $n = 1$ and for the first four angular momentum channels, i.e., $j = 1/2, 3/2$ and $j = -1/2, -3/2$. It is easily seen that topological defect and tilted magnetic field how can change the level splitting.

In conclusion, we have obtained the analytical bound states solutions of the Dirac equation in the presence of tilted magnetic field background using a particular symmetric and Landau gauges. When a graphene sheet is subjected to a magnetic field normal to the graphene surface, as well, is exposed to in-plane magnetic field the orbital motion of electrons is affected. Additionally, inclusion of together with topological defects in graphene sheet yield to distinct electronic properties. This kind of defects give rise to long-range modifications in the electronic wave function that affect the electronic spectrum which differs from produced by vacancies or other impurities modeled by local potentials.

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