Physics Letters A ••• (••••) •••–•••

Contents lists available at ScienceDirect

Physics Letters A

www.elsevier.com/locate/pla

# Nonlinearity of the zigzag graphene nanoribbons with antidots via the f-deformed Dirac oscillator in (2+1)-dimensions

M.R. Setare, P. Majari *

*Department of Science, University of Kurdistan, Sanandaj, Iran*

ARTICLE INFO

*Article history:*
Received 18 November 2017
Received in revised form 6 December 2017
Accepted 7 December 2017
Available online xxxx
Communicated by R. Wu

*Keywords:*
Graphene
F-deformation
Nonlinearity
Landau levels
Zigzag graphene nanoribbons

ABSTRACT

We study the nonlinearity for the zigzag graphene nanoribbons (ZGNRs) with zigzag triangular holes (ZTHs). We show that in the presence of an external uniform magnetic field, a two-dimensional f-deformed Dirac oscillator can be used to describe the dynamics of the electrons in the ZGNRs with ZTHs. It is shown for the first time that the magnetic field direction has effect on the chirality of charge carriers in the ZGNRs punched with triangular holes. We also obtain the Landau-level spectrum in the weak and strong magnetic field regimes. Additionally, we compare Landau-level spectrum of this graphene-based device in the f-deformed scenario and original one. Our results provide a general viewpoint for the development of the zigzag graphene nanoribbons.



## 1. Introduction

Graphene was the missing allotrope of pure carbon materials, after the discovery of graphite, diamond, fullerenes and carbon nanotubes (CNTs). In 2004, graphene, the youngest of the carbon allotropes, was discovered at the centre for Mesoscopic and Nanotechnology of the University of Manchester in the United Kingdom [1]. Structurally, graphene is defined as a two-dimensional crystal comprised of a one-atom thick layer of carbon atoms that are arranged in a honeycomb crystal lattice. Furthermore, it also exhibits very unique properties: one-atom thickness, remarkable mechanical strength, and high thermal and electrical conductivity [2–4]. So, the graphene is one of the subjects under the active research. While we usually describe the behavior of charge carriers in conventional materials with the Schrödinger equation, the interacting electrons in graphene are characterized by massless and relativistic Dirac fermions, which are moving through the honeycomb lattice with a velocity $v_f$ which is 300 times less than that of light [5]. Graphene is a zero-gap semiconductor, hence it cannot be directly used as an alternative to silicon in semiconductor electronics. The bandgap opening can be done when graphene lies on Boron nitride substrate. In this case, a small gap of a few meV is observed [6–8]. Also, one of the new candidates for band gap engineering applications is graphene nanoribbons (GNRs) [9,10]. In recent years, there has been growing interest in creating a graphene nanostructure from a bulk sample. Geometrically, the simplest nanostructures of graphene with a rectangular shape assumed to have a width typically smaller than 100 nm, are called graphene nanoribbons (GNRs). There are two basic edge shapes from many possible edge geometries, armchair and zigzag, which determine the properties of graphene ribbons [11,12]. Sufficiently narrow zigzag edge graphene nanoribbons show a bandgap which comes from a staggered sublattice potential due to spin ordered states at the edges [13,14]. Specially, graphene quantum dots and antidots are another kind of graphene nanostructures which have been gaining considerable interest in recent years. Here, we focused on graphene-based devices by combining ZGNRs and triangular antidots(holes) with zigzag edges. In Ribbons, the low-energy spectrum of the charge carriers can be studied with a Dirac Hamiltonian [15]. Therefore, the physics of charge carriers in a ZGNR with zigzag triangular holes is governed by the following Dirac-like equation:

$$i\hbar\frac{\partial|\psi>}{\partial t}=[\sum_{j=1}^{2}v_f\sigma_j p_j+\Delta\sigma_z]|\psi>, \tag{1}$$

where $\sigma_j$ and $\sigma_z$ are Pauli matrices, $\Delta$ and $p_j$ are, respectively, half of the induced gap in ZGNR spectra and j-component of the linear momentum [6,16]. From a theoretical perspective, the motion of

* Corresponding author.
*E-mail addresses:* rezakord@ipm.ir (M.R. Setare), maajari@gmail.com (P. Majari).

https://doi.org/10.1016/j.physleta.2017.12.015

the charge carriers relative to the planar hexagonal arrangement of carbon atoms in graphene is the source of internal magnetic field [17]. On the other hand, the intensity of this internal magnetic field is unknown and may be negligible. Only under certain conditions, such as punched zigzag-edged triangular-shaped graphene structures or graphene doped with other elements, do internal magnetic fields play an impressive role in the systems' dynamics. So, we focus on the zigzag graphene nanoribbons with ZTHs. Two possible magnetic states of zigzag-edged nanoribbon are antiferromagnetic one in which spins have opposite directions on opposite edges and the ferromagnetic one with the same directions [18]. In addition, the three edges in the triangle holes have ferromagnetic states. So, punched zigzag-edged triangular-shaped graphene nanoribbons display unique ferromagnetic order. "The ferromagnetic coupling between the edge states on the triangular hole leads to a finite total magnetic moment" [19]. This finite total magnetism sets up an effective internal magnetic field $\vec{B}_{int} = -B_{int} e_z$. The vector potential in the symmetric gauge for this magnetic field can be chosen as $A_{int} = (\frac{B_{int}}{2} y, \frac{-B_{int}}{2} x, 0)$. In this case, charge carriers feel the magnetic field. So, our momentum changes to the canonical momentum. As a consequence, the Eq. (1) for this vector potential becomes as follows:

$$i\hbar\frac{\partial|\psi>}{\partial t} = [\sum_{j=1}^{2} v_f \sigma_j (p_j + \frac{e}{c} A_{j,int}) + \Delta\sigma_z]|\psi>, \tag{2}$$

where $c$ is the speed of light and e denotes the electron charge. Then, the corresponding Hamiltonian can be written as:

$$\hat{H} = \begin{bmatrix} \Delta & v_f[p_x + i\frac{B_I e x}{4} - ip_y + \frac{B_I e y}{4}] \\ v_f[p_x - i\frac{B_I e x}{4} + ip_y + \frac{B_I e y}{4}] & -\Delta \end{bmatrix}, \tag{3}$$

where $B_I = 2B_{int}$, also we use the units such that $c = 1$. A straightforward calculation shows that the above Hamiltonian is equivalent with the Dirac oscillator Hamiltonian, as:

$$H = \sum_{j=1}^{2} v_f \sigma_j (p_j - i\frac{eB_I}{4}\sigma_z r_j) + \Delta\sigma_z, \tag{4}$$

which $(-i\frac{eB_I}{4}\sigma_z r.\sigma)$ can be interpreted as the linear potential in the (2+1)-dimensional Dirac oscillator [17]. So, the behavior of electrons in a ZGNR with zigzag triangular holes can be described by a (2+1)-dimensional Dirac oscillator.[1]

An important property of graphene which has attracted considerable interest, especially within recent years, is its nonlinearity. The nonlinear optical response of graphene in a strong magnetic field, where the resulting magnitude of the third-order nonlinear susceptibility $\chi^{(3)}$ turns out to be extremely large, is discussed in [21]. "Graphene in the presence of an external magnetic field shows a nonlinearity originating from its unusual band structure and selection rules for the optical transitions near the Dirac point" [21]. To investigate the effect of this nonlinearity in ZGNR, we study the (2+1)-dimensional f-deformed Dirac oscillator [22]. The f-oscillator is a nonlinear oscillator with a specific kind of nonlinearity for which the frequency depends on the oscillation energy. In the general form, we can represent this dependency with a function f [23].

In this paper, we study the ZGNR with zigzag triangular holes in the presence of an external magnetic field in a f-deformed scenario. The paper is organized as follows. In Section 2, we study the f-deformed Hamiltonian for ZGNR punched with triangular holes in a homogeneous and constant magnetic field. By applying an external magnetic field, parallel and anti-parallel with the internal magnetic field, we discuss about different chirality for the charge carriers. Then, in Section 3, we study the effects of the magnetic field strength on our graphene-based device. Finally, in section 4 we discuss and conclude our results.

## 2. The f-deformed Hamiltonian in ZGNR with zigzag triangular holes

As mentioned in the introduction, a ZGNR with zigzag triangular holes can be described by the (2+1)-dimensional Dirac oscillator. In this section, we want to describe the dynamics of charge carriers of our graphene-based device with the two-dimensional Dirac oscillator. After introduction of the formal change $\Delta \to m{v_f}^2$, Eq. (4) can be written in the form of the following two-dimensional Dirac oscillator:

$$i\hbar\frac{\partial|\psi>}{\partial t} = [\sum_{j=1}^{2} v_f \sigma_j (p_j - i\frac{eB_I}{4}\sigma_z r_j) + m{v_f}^2\sigma_z]|\psi>, \tag{5}$$

where m is the effective mass. "The ferromagnetic coupling between the edge states on the triangular hole leads to a finite total magnetic moment. This finite total magnetism sets up $B_I$" [19]. Now, we consider the problem of an external uniform magnetic field B applied perpendicular to the ZGNR plane ($\vec{B} = B\hat{e}_z$) with corresponding vector potential $A$. The vector potential in the symmetric gauge for this magnetic field can be chosen as $A = (\frac{-B}{2}y, \frac{B}{2}x, 0)$. In the presence of an external magnetic field, $p_j$ in the above equation should be replaced with $p_j \to p_j + \frac{e}{c}A_j$. Then Eq. (5) takes the following form:

$$i\hbar\frac{\partial|\psi>}{\partial t} = [\sum_{j=1}^{2} v_f \sigma_j (p_j - i\frac{eB_I}{4}\sigma_z r_j + eA_j) + m{v_f}^2\sigma_z]|\psi>. \tag{6}$$

The internal magnetic field introduces a new length scale, the magnetic length ${l_B}^2 = \frac{\hbar}{eB_I}$. Next, we introduce the so-called cyclotron frequency $\omega_c$ defined by ${\omega_c}^2 = \frac{eB{v_f}^2}{\hbar}$. Then, the Hamiltonian of ZGNR punched with triangular holes is given by:

$$\hat{H} = \begin{bmatrix} m{v_f}^2 & v_f[p_x + i\frac{\omega^2\hbar}{{v_f}^2}x - i\frac{\tilde{\omega}^2\hbar}{{v_f}^2}x - ip_y + \frac{\omega^2\hbar}{{v_f}^2}y - \frac{\tilde{\omega}^2\hbar}{{v_f}^2}y] \\ v_f[p_x - \frac{i\omega^2\hbar}{{v_f}^2}x + \frac{i\tilde{\omega}^2\hbar}{{v_f}^2}x + ip_y + \frac{\omega^2\hbar}{{v_f}^2}y - \frac{\tilde{\omega}^2\hbar}{{v_f}^2}y] & -m{v_f}^2 \end{bmatrix}, \tag{7}$$

where we have used the substitutions $\omega^2 = \frac{{v_f}^2}{4{l_B}^2}$ and $\tilde{\omega}^2 = \frac{{\omega_c}^2}{2}$. Now, we want to express our Hamiltonian in the term of chiral creation and annihilation operators. For this purpose, we introduce two different types of chiral annihilation operators. The chiral annihilation operators for the frequency $\omega$, are given by [24]:

$$a_l = \frac{1}{\sqrt{2}}(a_x + ia_y) = \frac{iv_f}{2\sqrt{2}\omega\hbar}[(p_x - \frac{2i\hbar\omega^2 x}{{v_f}^2}) + i(p_y - \frac{2i\hbar\omega^2 y}{{v_f}^2})], \tag{8}$$

and

[1] The Dirac oscillator was introduced by Moshinsky and Szczepaniak in 1989 [20]. They considered a new type of interaction in an attempt to describe a relativistic oscillator by means of a Dirac equation linear in both momentum and coordinates.

Please cite this article in press as: M.R. Setare, P. Majari, Nonlinearity of the zigzag graphene nanoribbons with antidots via the f-deformed Dirac oscillator in (2+1)-dimensions, Phys. Lett. A (2018), https://doi.org/10.1016/j.physleta.2017.12.015