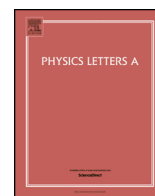


Contents lists available at [ScienceDirect](http://ScienceDirect.com)

Physics Letters A

www.elsevier.com/locate/pla

Bound states in disclinated graphene with Coulomb impurities in the presence of a uniform magnetic field

J.F.O. de Souza^a, C.A. de Lima Ribeiro^b, Claudio Furtado^{a,*}^a Departamento de Física, CCEN, Universidade Federal da Paraíba, Cidade Universitária, 58051-970 João Pessoa, PB, Brazil^b Departamento de Física, Universidade Estadual de Feira de Santana, Novo Horizonte, 44036-900 Feira de Santana, BA, Brazil

ARTICLE INFO

Article history:

Received 21 February 2014
Received in revised form 2 May 2014
Accepted 5 May 2014
Available online 5 June 2014
Communicated by V.M. Agranovich

Keywords:

Coulomb Impurity
Gapped Graphene
Massive Dirac excitation
Topological defect

ABSTRACT

In this contribution, we study the effects caused by an impurity on the quantum dynamics of massive excitations in a disclinated graphene in the presence of an external magnetic field. Within a continuum approach, the problem is mathematically modeled by the definition of a special vector potential containing all the information about the topology and the interacting fields. The presence of disclination is introduced by a term in the Dirac equation that translates the appearance of a phase associated with the transport of the spinor around the apex of the cone. We solve exactly the Dirac equation for this problem and the eigenvalues are obtained. We observe the influence of the disclination on the spectrum of energy and the allowed values of magnetic field.

Crown Copyright © 2014 Published by Elsevier B.V. All rights reserved.

1. Introduction

Physical systems of low dimensionality have attracted a considerable attention in recent years, especially after the synthesis in 1991 of carbon nanotubes, which behave like one-dimensional structures [1]. In 1997, the graphite cones were obtained experimentally by Krishnan et al. [2]. A lot of topological effects were found in the structures produced from them. It was thought that it would be impossible to produce a two-dimensional crystalline solid. Landau, in 1937, proposed a theory in which the temperature itself could create instability in the structure, which caused its break [3]. The formation of thin films with thickness each time smaller caused the decrease of the melting temperature of the sample implying it to be unstable [4,5]. In 2004, the synthesis of graphene gave rise to a surprising and relevant change from the conceptual point of view [6]. Graphene is a flat sheet composed of carbon atoms arranged in a two-dimensional honeycomb lattice (see Fig. 1).

Before its synthesis, however, the presence of topological defects in graphene was treated [7]. It was shown that electronic structure, transport properties and some other related physical aspects are significantly altered for cones fabricated from graphite layers. A carbon nanocone can be regarded as a system with a topological defect known as disclination. Disclination in graphene

is formed from the removal or addition of an angular sector of the two-dimensional hexagonal lattice. The angle deficit generates a positive disclination, and leaves the apex of the cone with a number of ring atoms proportional to the removed section. Disclinations in graphene have been treated in the literature within some theoretical approaches [8]. Particularly, the low-energy limit has attracted an enormous interest. At low energies, the quantum behavior of excitations in graphene is governed by an equation analogous to a two-dimensional massless Dirac equation. These excitations behave as massless relativistic particles with a Fermi velocity of approximately 10^6 m/s. In the absence of sublattice symmetry, a gap appears and the corresponding dynamics can be incorporated by a massive term in this equation, i.e., quantum dynamics will be described by considering massive relativistic particles. Graphene grown on a SiC substrate is a good example of this situation. It is a known fact that a band gap is induced in these samples and massive Dirac fermions play a central role in the low-energy limit [9]. In general, this case is called gapped graphene. Here, we shall deal with this specific case. A more elaborated presentation is given in the next section.

González, Guinea and Vozmediano [10,11] proposed a theoretical model for fullerene molecules based on the insertion of combined topological defects. A Dirac description was employed to describe a fullerene molecule subjected to a radial magnetic field in order to find some agreement with parallel numerical results. In this model, the presence of the field is used to simulate the effective topological effects on the system. In 2000, Lammert and Crespi [7] used a similar low-energy approach and started to study

* Corresponding author. Tel.: +55 83 3216 7534.

E-mail addresses: jfernando@fisica.ufpb.br (J.F.O. de Souza), calr@uefs.br (C.A. de Lima Ribeiro), furtado@fisica.ufpb.br (C. Furtado).

the electronic behavior of disclinated monolayers of graphite with conical geometry. Meanwhile, alternative analytical methods in self-consistent field-theory models were also used in order to study the electronic structure of graphitic cones. Osipov, Kochetov and Pudlak [12–14] obtained the local and total density of states near the defects for these and other disclinated systems. In 2004, Lammert and Crespi [15] proposed a classification of general graphene cones with two-pentagon disclinations by considering the type of fictitious gauge flux. Investigations about the influence of topological defects and local curvature on flat graphene systems were also made by Cortijo and Vozmediano [16–18]. Although the characteristic linear dispersion is known since Wallace [19], the traditional continuum formulation in terms of a Dirac equation, present in each one of the above mentioned works, acquired notability with the effective-mass approximation used by Di Vincenzo and Mele [20] within a treatment for graphite compounds in the presence of single intercalants. Not only these works, but also other remarkable contributions have helped us to elucidate the mechanisms by which disclinations can affect the physics of a graphene layer. Nowadays, unexplored physical configurations and phenomena have guaranteed a constant theoretical interest in disclinated graphitic systems. Their peculiar topological effects are still expected to produce relevant physical properties and promising applications in future.

The usual low-energy description for a disclinated graphene encoding the conical topology consists of defining a vector potential and putting it into the Dirac Hamiltonian. This term inserts the typical behavior of the spinor when transported around the apex of the cone, i.e., it describes the appearance of a phase. Although this phase does not arise from a real physical interaction, it can be modeled as an Aharonov–Bohm phase [7,15,21]. An extended approach applied to a system with multiple cones can be achieved by the introduction of an effective defect [21]. Recently, geometric approaches have been employed to investigate global aspects of the quantum behavior of Dirac particles under influence of disclinations in graphene. Several recent contributions can be found in the literature [21–24]. A good review on applications of gauge fields in graphene is presented in Ref. [25].

Coulomb impurities appeared for the first time in this environment within models for carrier transport in graphene. Experimental results suggested particular and interesting properties related to the electronic transport in this material, such as a minimum value for conductivity near the Dirac point, where the number of particles goes to zero, and its linear relation with the gate voltage and the density of carriers [6,26]. These discoveries led to the first theoretical treatments modeling transport in graphene by taking charged impurities as dominant scatters [27,28]. In recent works, Coulomb impurities have been shown to play an important role on transport phenomena in graphene sheets with topological defects. Not only the influence of impurities and topological defects on scattering of electrons in a low-energy regime, but also effects on properties of bound states in the gapped case have been investigated in these systems [29,30]. It is known that a fundamental point of the Coulomb impurity problem in graphene is the existence of a critical charge which separates two different regimes depending on the Coulomb strength [31]; various relevant aspects related to this point have been treated [32–35]. In this context, disclinated (gapped) graphene is found to exhibit important physical distinctions between subcritical and supercritical behaviors [29,30].

The electronic properties of gapped and gapless graphene subjected to a homogeneous magnetic field in the presence of a Coulomb impurity were investigated in Ref. [36]. The authors have employed variational methods to study this problem in a Dirac formulation; the eigenfunctions of Landau levels in graphene are used as trial wave functions and the spectrum of eigenvalues for

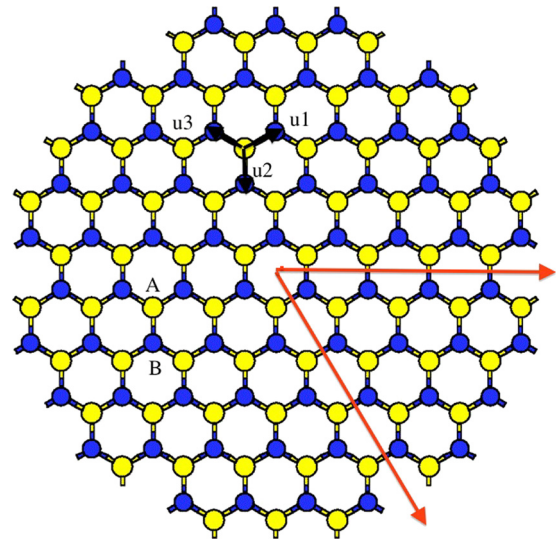


Fig. 1. Two-dimensional honeycomb lattice viewed as two intertwined triangular sublattices. Sublattices *A* and *B* are represented by yellow and blue sites, respectively. The vectors \vec{u}_1 , \vec{u}_2 and \vec{u}_3 connect the sites *A* to their first neighbors. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

the impurity problem is constructed from them. Recently, numerical calculations based on a series method have revealed significant details about the behavior of Dirac states in the same background [37].

The Landau levels for a graphene layer in the presence of topological defects were studied in [15,38]. Lammert and Crespi [15] investigated the electronic states for a massless graphene cone interacting with a uniform magnetic field. A dependence on the parameter that describes the topology was found in Landau levels. In this article, we study the effects caused by charged impurities in the presence of an external uniform magnetic field on a gapped graphene in subcritical case. We check the role of a disclination in this system.

This paper is organized as follows. In Section 2, we present the formalism adopted in this work, where the mathematical scenario for a gapped graphene is briefly characterized. In Section 3, we take an already established background for gapped graphene cones with charge impurities and, by introducing an extra term in order to incorporate the magnetic field, we construct the Hamiltonian for the problem. We also obtain the analytical solutions for asymptotic limits, which allows us to write our *Ansatz*. In Section 4, we solve the Dirac equation by the Frobenius method and find the eigenvalues and the allowed values of magnetic field. The conclusions are presented in Section 5.

2. Dirac equation for a massive graphene

Graphene is a monolayer of graphite. It consists of carbon atoms which form a honeycomb lattice. This lattice can be considered as two intertwined triangular lattices (see Fig. 1). The σ bonds are formed from orbitals in a configuration sp^2 hybridized. These are links that provide stability to the structure of graphene. The π bonds cause the valence and conduction bands. We can describe the electronic properties near the Fermi energy by a tight-binding model. This model is characterized by two points usually called Dirac points, and the effective Hamiltonian is linear in momentum, when we are close to them. Recently, many investigations on the influence of presence of various impurities, electron–electron interactions and substrate structures which are responsible for appearance of a mass gap in graphene have been carried out [32,37,39–54]. These effects are responsible for break-

ing of sublattice symmetry leading to a mass gap in a graphene layer.

The Hamiltonian describing the π carbon orbitals in a gapped graphene is given by

$$\mathcal{H} = t \sum_{i=A} \sum_{j=1}^3 [a^\dagger(\vec{r}_i) b(\vec{r}_i + \vec{u}_j) + b^\dagger(\vec{r}_i + \vec{u}_j) a(\vec{r}_i)] + \beta \sum_{i=A} [a^\dagger(\vec{r}_i) a(\vec{r}_i) - b^\dagger(\vec{r}_i + \vec{u}_j) b(\vec{r}_i + \vec{u}_j)], \quad (1)$$

where t expresses the probability of transition by tunneling and yields ≈ -3 eV for graphene, and 2β is the energy difference of electrons on sites A and B . For gapless graphene one has $\beta = 0$. The creation and annihilation operators create and annihilate electrons in their respective sublattices, i.e., a and a^\dagger act on the sublattice A , while b and b^\dagger on the sublattice B . The vectors \vec{u}_1, \vec{u}_2 and \vec{u}_3 connect the sites A to the first neighbors.

We change the representation from the real space to that one in the reciprocal space via the Fourier transform:

$$a(\vec{r}_i) = \frac{1}{\sqrt{N}} \sum_{\vec{k}} e^{i\vec{k}\cdot\vec{r}_i} \tilde{a}(\vec{k}); \quad (2a)$$

$$b(\vec{r}_{i'}) = \frac{1}{\sqrt{N}} \sum_{\vec{k}} e^{i\vec{k}\cdot\vec{r}_{i'}} \tilde{b}(\vec{k}), \quad (2b)$$

where $\vec{r}_{i'} = \vec{r}_i + \vec{u}_j$ and N is the number of sites A (or B). We obtain the Hamiltonian:

$$\mathcal{H} = \sum_{\vec{k}} (\tilde{a}^\dagger(\vec{k}) \tilde{b}^\dagger(\vec{k})) \begin{pmatrix} \beta & t \sum_{j=1}^3 e^{i\vec{k}\cdot\vec{u}_j} \\ t \sum_{j=1}^3 e^{-i\vec{k}\cdot\vec{u}_j} & -\beta \end{pmatrix} \times \begin{pmatrix} \tilde{a}(\vec{k}) \\ \tilde{b}(\vec{k}) \end{pmatrix}, \quad (3)$$

where we have rewritten the expression for the first Brillouin zone in the reciprocal space. We solve the eigenvalue problem, diagonalizing the matrix inside the sum and using $\Psi = \begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix}$ as an eigenvector. The corresponding eigenvalues are:

$$E^2 = \beta^2 + t^2 \left| \sum_{j=1}^3 e^{i\vec{k}\cdot\vec{u}_j} \right|^2. \quad (4)$$

An appropriate choice of orientation allows us to arrive at

$$E = \pm \left(\beta^2 + t^2 \left[3 + 2 \cos(\sqrt{3}k_y d) + 4 \cos\left(\frac{3}{2}k_x d\right) \cos\left(\frac{\sqrt{3}}{2}k_y d\right) \right] \right)^{1/2}, \quad (5)$$

with d the distance between carbon atoms in the lattice. In it we can find two surfaces: one of them has a negative energy (valence band) filled with states, and the other one has a positive energy (conduction band) with empty states. As the energy eigenvalues have minimum at the corners of the Brillouin zone, the separation between the two bands becomes minimal at the corners. This degeneration occurs at six points located at the vertices of the first Brillouin zone in the form of a hexagon. Each of them forms, separately, the Fermi surface of graphene, and therefore they are called the Fermi points. We consider the case when the six points are reduced to only two, which we call \vec{K} and \vec{K}' . For small momenta near these points, we reach the continuum limit, where electrons

are found to show a Dirac-like behavior. In this limit, the Hamiltonian assumes the following form

$$\mathcal{H} = \sum_{\vec{q}} [\Psi^\dagger(\vec{q}) (v_F \vec{\sigma} \cdot \vec{q} + v_F^2 m \sigma^3) \Psi(\vec{q})], \quad (6)$$

where $\vec{q} = (q_x, q_y)$ is the momentum relative to the Dirac point \vec{K} , $v_F = \frac{3td}{2}$ is the Fermi velocity, $m = \frac{\beta}{v_F}$ and σ matrices obey the Dirac algebra $\{\sigma^\mu, \sigma^\nu\} = 2\eta^{\mu\nu}$. Therefore, in the low-energy limit, the gap will be represented by a massive term in a Dirac-like equation. In the case $\beta = 0$, we have the massless graphene limit. In this work, we shall consider a Dirac excitation in a gapped background. Then, back to the real space by a new Fourier transform, the behavior of our system will be described by the following equation:

$$(-i\sigma^\mu \partial_\mu + m\sigma^3) \psi(\vec{r}) = E\psi(\vec{r}), \quad (7)$$

where $\vec{\sigma} = (\sigma^1, \sigma^2, \sigma^3)$ are the Pauli matrices and E is the energy; here we have taken $v_F = 1$. For more details on the tight-binding formulation for graphene, see Refs. [19,55,56].

3. Massive fermion in the background of a topological defect in the presence of charged impurity and uniform magnetic field

Now, we suppose the presence of electromagnetic and topological fields and add the interactions between fields and massive fermions by introducing the minimal coupling into the Dirac equation. More precisely, we implement the following coupling:

$$q^\mu \longrightarrow q^\mu - eA^\mu, \quad (8)$$

where $A^\mu = (\phi, \vec{A})$ is the 4-vector potential. It thus formally features the insertion of fields within the relativistic quantum mechanics and, more particularly, in graphene. In our particular case, as will be shown, the problem is characterized via the definition of a special 4-vector potential responsible for containing all the information about the topology and interactions with external fields.

From a topological point of view, disclinations can be obtained by a transformation known as Volterra process [57]. By cutting and removing a sector, from a flat graphene sheet we construct a disclination gluing the new edges, as shown in Figs. 2a and 2b. The removed angular sector must be a multiple n of 60° . Following the procedure of Lammert, Crespi and other authors [7,17,21,29], we incorporate the topological defect in the medium by introducing a specific vector potential which can reproduce the already known effect of the conical topology on the behavior of the spinor [7,21]. As is well known, in practice, the topological aspect of the cone is manifested by the appearance of a phase in the Dirac spinor. The effective transport of the Dirac spinor around the apex corresponds to a holonomy transformation which, for an arbitrary n -disclination, yields a phase given by [29]

$$\psi(r, \theta + 2\pi) = e^{i2\pi[\pm\frac{n}{4}\sigma^0 + (1-\frac{n}{6})\frac{\sigma^3}{2}]} \psi(r, \theta), \quad (9)$$

where n is the number of sectors removed from the plane from which we construct the cone and σ^0 is the matrix identity. For a detailed description of the mathematical background, see the above named references. This phase can be considered as a phase of the Aharonov–Bohm effect derived from the presence of a fictitious flux, which allows us to model the effect of disclination by defining the vector potential given by:

$$\vec{A} = \frac{1}{er} \left[\pm \frac{n}{4} \sigma^0 + \frac{\sigma^3}{2} \right] \hat{\theta}. \quad (10)$$

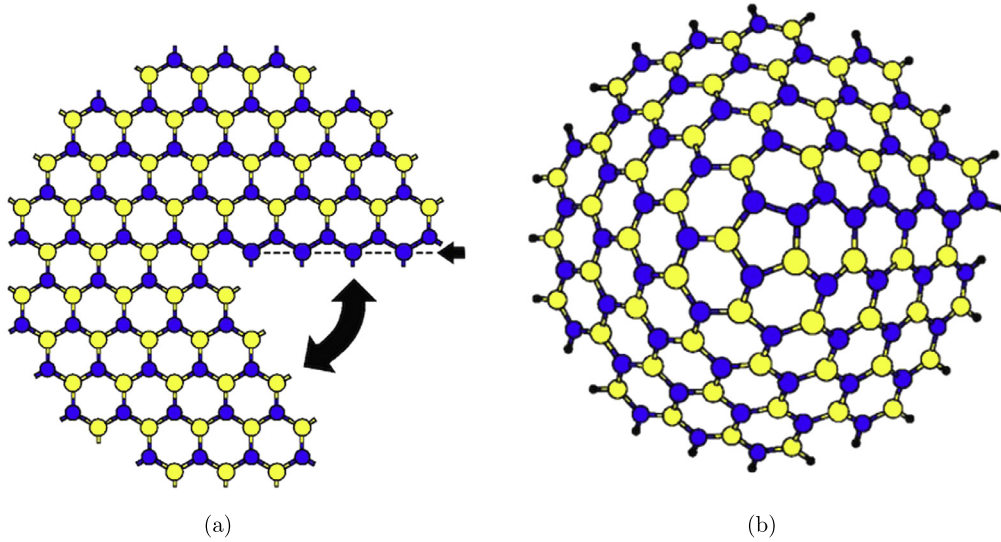


Fig. 2. (a) Cutting and removing an angular sector of 60° from the original lattice, corresponding to a disclination with $n = 1$. (b) Creation of a disclination with a pentagon at its apex obtained by gluing the new edges.

Therefore, to introduce the effect of the topology of the cone into the physical description of our system based on graphene, we must couple this vector potential within the Dirac equation (7).

Let us now introduce a uniform magnetic field into the system. Taking a perpendicular field as $\vec{B} = B\hat{z}$, we can model the graphene cone by introducing an extra term to the vector potential (10), in the following form

$$\vec{A}_m = \frac{1}{2} Br \hat{\theta}. \quad (11)$$

This is the term responsible for incorporating the uniform magnetic field in the system. Then we redefine the potential (10) as:

$$\vec{A} = \frac{1}{er} \left[\pm \frac{\frac{n}{4} \sigma^0}{(1 - \frac{n}{6})} + \frac{\sigma^3}{2} + \frac{1}{2} eBr^2 \right] \hat{\theta}. \quad (12)$$

In this way, this effective vector potential incorporates all contributions to this fermionic dynamics; the influence of the geometry of the topological defect is represented by first two terms in (12), and the last one emerges due to the external uniform magnetic field.

Now we consider the Dirac equation for a gapped graphene in the presence of the external potential (12). It is given by

$$[\sigma^\mu (-i\partial_\mu - eA_\mu) + m\sigma^3] \Psi(t, r, \theta) = 0, \quad (13)$$

where ∂_μ is the usual derivative in the coordinate system associated with the disclinated graphene. Then, we implement the influence of a charged impurity localized at the apex of the gapped graphene cone [29,30], which is given by

$$U(r) = -\frac{\alpha}{r}, \quad (14)$$

where $\alpha = \frac{Ze^2}{\hbar v_F \kappa}$ is the Coulomb interaction strength, Z is the atomic number and κ is the dielectric constant. Finally, taking into account the term which corresponds to the Coulomb interaction by coupling it as a time-like component, we write the Dirac equation as

$$\begin{pmatrix} m - \frac{\alpha}{r} - E & \partial_r - \frac{i}{r(1-\frac{n}{6})} \partial_\theta \pm \frac{\frac{n}{4}}{r(1-\frac{n}{6})} + \frac{1}{2r} - \frac{1}{2} eBr \\ -\partial_r - \frac{i}{r(1-\frac{n}{6})} \partial_\theta \pm \frac{\frac{n}{4}}{r(1-\frac{n}{6})} - \frac{1}{2r} - \frac{1}{2} eBr & -m - \frac{\alpha}{r} - E \end{pmatrix} \times \begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix} = 0. \quad (15)$$

We consider the solution of the form

$$\psi(r, \theta) = \sum_j \begin{pmatrix} R_A^{(j)}(r) \\ R_B^{(j)}(r) \end{pmatrix} e^{ij\theta}, \quad (16)$$

where the total angular momentum j takes all half integer values $j = 0, \pm 1/2, \pm 3/2, \pm 5/2, \dots$. Now, we consider asymptotic limits $r \rightarrow 0$ and $r \rightarrow \infty$ for Eq. (15). For small r , the radial equation reduces to the following one:

$$\frac{d^2 R_{A(B)}}{dr^2} + \frac{2}{r} \frac{dR_{A(B)}}{dr} - \frac{1}{r^2} \left(\gamma^2 - \frac{1}{4} \right) R_{A(B)} = 0, \quad (17)$$

where

$$\gamma = \sqrt{v^2 - \alpha^2}, \quad v = \frac{(j \pm \frac{n}{4})}{(1 - \frac{n}{6})}. \quad (18)$$

The solution of Eq. (17) in a short distance limit is given by:

$$R_{A(B)} \sim r^{\gamma - \frac{1}{2}}. \quad (19)$$

At this moment, it is interesting to notice that $|\alpha|$ could overcome $|v|$. In this case γ becomes imaginary. The solutions for the eigenstates will become uncontrollably oscillatory and will have no well defined limit when r goes to zero. For this contribution, we suggest that the parameter γ is in the subcritical regime, i.e., $v^2 > \alpha^2$. Solutions $R_{A(B)}$ reveal, in this regime, the same behavior for the case without the magnetic field described in Ref. [29], as expected. On the other hand, for a very large r , the equation takes the form

$$\frac{d^2 R_{A(B)}}{dr^2} + \frac{2}{r} \frac{dR_{A(B)}}{dr} - \frac{1}{4} (e^2 B^2 r^2) R_{A(B)} = 0, \quad (20)$$

and its solution behaves as

$$R_{A(B)} \sim e^{-\frac{eB}{4} r^2}. \quad (21)$$

Here we eliminate the exponentially increasing solution imposing a normalizability condition for the solution. As we can observe, we have the same behavior found in the massless case without Coulomb field [15].

4. Solutions of the Dirac equation

In this section, we find the eigenvalues and eigenfunctions for this problem. As we saw in the previous section, the system in question is described by the following Hamiltonian:

$$H = \begin{pmatrix} m - \frac{\alpha}{r} & \partial_r - \frac{i}{r(1-\frac{\eta}{6})} \partial_\theta \pm \frac{\frac{\eta}{4}}{r(1-\frac{\eta}{6})} + \frac{1}{2r} - \frac{1}{2} eBr \\ -\partial_r - \frac{i}{r(1-\frac{\eta}{6})} \partial_\theta \pm \frac{\frac{\eta}{4}}{r(1-\frac{\eta}{6})} - \frac{1}{2r} - \frac{1}{2} eBr & -m - \frac{\alpha}{r} \end{pmatrix}. \tag{22}$$

In the Hamiltonian (22) we have introduced, simultaneously, the effect of the topology of the disclination, the Coulomb interaction and the uniform magnetic field. So, we must solve the following Dirac equation:

$$\begin{pmatrix} m - \frac{\alpha}{r} - E & \partial_r - \frac{i}{r(1-\frac{\eta}{6})} \partial_\theta \pm \frac{\frac{\eta}{4}}{r(1-\frac{\eta}{6})} + \frac{1}{2r} - \frac{1}{2} eBr \\ -\partial_r - \frac{i}{r(1-\frac{\eta}{6})} \partial_\theta \pm \frac{\frac{\eta}{4}}{r(1-\frac{\eta}{6})} - \frac{1}{2r} - \frac{1}{2} eBr & -m - \frac{\alpha}{r} - E \end{pmatrix} \times \begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix} = 0. \tag{23}$$

To do this, we will search for the solution of (23) in the form of the following Ansatz

$$\begin{cases} \psi_A = R_A e^{ij\theta} \\ \psi_B = R_B e^{ij\theta}. \end{cases} \tag{24}$$

Substituting (24) into (23), we arrive at the following system of equations

$$\begin{cases} \left(m - \frac{\alpha}{r} - E \right) R_A + \left[\frac{d}{dr} + \frac{j}{r(1-\frac{\eta}{6})} \pm \frac{\frac{\eta}{4}}{r(1-\frac{\eta}{6})} + \frac{1}{2r} - \frac{1}{2} eBr \right] R_B = 0 \\ \left[-\frac{d}{dr} + \frac{j}{r(1-\frac{\eta}{6})} \pm \frac{\frac{\eta}{4}}{r(1-\frac{\eta}{6})} - \frac{1}{2r} - \frac{1}{2} eBr \right] R_A + \left(-m - \frac{\alpha}{r} - E \right) R_B = 0. \end{cases} \tag{25}$$

Now, we consider the asymptotic behavior of the solutions $R_A(r)$ and $R_B(r)$ previously found in Section 3, suggesting for them the following Ansatz:

$$R_A(r) = e^{-\frac{eB}{4}r^2} r^{\gamma-\frac{1}{2}} F(r) \tag{26}$$

and

$$R_B(r) = e^{-\frac{eB}{4}r^2} r^{\gamma-\frac{1}{2}} G(r). \tag{27}$$

We want to find differential equations for the functions $F(r)$ and $G(r)$. Substituting (26) and (27) into (25), we arrive at the following equations:

$$rF'(r) - (\gamma - \nu)F(r) + [(m + E)r - \alpha]G(r) = 0, \tag{28}$$

and

$$rG'(r) + (\gamma + \nu - eBr^2)G(r) + [(m - E)r - \alpha]F(r) = 0. \tag{29}$$

We can find G from (28) and, substituting it into (29), we obtain the equation that must be satisfied by the function F :

$$r^2 F''(r) + \left[-\left(\frac{m + E}{(m + E)r + \alpha} \right) r^2 + c_1 r + c_2 r^3 \right] F'(r) + \left[-\left(\frac{(m + E)(\gamma - \nu)}{(m + E)r + \alpha} \right) r + c_3 r^2 + c_4 r \right] F(r) = 0, \tag{30}$$

where we defined $c_1 = 2\gamma + 1$, $c_2 = -eB$, $c_3 = -[(\gamma - \nu)eB + m^2 - E^2]$ and $c_4 = 2E\alpha$. We can rewrite (30) in a more tractable form

by making the change of variable $u = \left(\frac{m+E}{\alpha} \right) r$. This change leads to the equation

$$u^2 F''(u) + \left[-\frac{1}{(1+u)} u^2 + k_1 u + k_2 u^3 \right] F'(u) + \left[\frac{k_3}{(1+u)} u + k_4 u^2 + k_5 u \right] F(u) = 0, \tag{31}$$

with $k_1 = c_1$, $k_2 = \frac{\alpha^2}{(m+E)^2} c_2$, $k_3 = -(\gamma - \nu)$, $k_4 = \frac{\alpha^2}{(m+E)^2} c_3$ and $k_5 = \frac{\alpha}{m+E} c_4$. Eq. (31) apparently cannot be reduced to a known solution. Therefore, we must find a solution directly by applying the Frobenius theorem, from which we know that around a regular singular point u_0 , there is at least one solution in the form:

$$F(u) = \sum_{\bar{n}=0}^{\infty} C_{\bar{n}} (u - u_0)^{\bar{n}+\delta}, \tag{32}$$

where δ is a constant to be determined. Thus, we assume such a solution with $u_0 = 0$, one regular singular point of Eq. (31), and we replace it in order to determine the value of δ and the relations among the coefficients $C_{\bar{n}}$. After this, we find the following relationship:

$$\begin{aligned} & [(\bar{n} + \delta + 3)(\bar{n} + \delta + 2) + k_1(\bar{n} + \delta + 3)] C_{\bar{n}+3} \\ & + [(\bar{n} + \delta + 2)(\bar{n} + \delta + 1) - (\bar{n} + \delta + 2) \\ & + k_1(\bar{n} + \delta + 2) + k_3 + k_5] C_{\bar{n}+2} + [k_2(\bar{n} + \delta + 1) + k_4 + k_5] \\ & \times C_{\bar{n}+1} + [k_2(\bar{n} + \delta) + k_4] C_{\bar{n}} = 0, \end{aligned} \tag{33}$$

where $\delta = 1 - k_1$, or $\delta = 0$, are the roots of the indicial equation.

The series must be truncated after a certain term to make the solution normalizable. Imposing this condition to the recurrence relation (33), we find:

$$k_2(\bar{n} + \delta) + k_4 = 0, \tag{34}$$

from which we obtain, for $\delta = 0$, the expression for the energy eigenvalues

$$E^2 = m^2 + (\bar{n} + \gamma - \nu)eB, \quad \bar{n} = 0, 1, 2, \dots \tag{35}$$

Substituting γ and ν into (35), we find the following eigenvalues

$$E^2 = m^2 + eB_{\bar{n}\nu} \left[\bar{n} + \sqrt{\left(\frac{j \pm \frac{\eta}{4}}{1 - \frac{\eta}{6}} \right)^2 - \alpha^2 - \frac{(j \pm \frac{\eta}{4})}{1 - \frac{\eta}{6}}} \right], \tag{36}$$

where $B_{\bar{n}\nu}$ are possible values of the magnetic field. Note that, in the limit $n = 0$, that is, absence of the topological defect, we obtain the results for a Dirac electron in the presence of Coulomb and uniform magnetic fields in (2 + 1) dimensions [58].

However, although we have found the energy eigenvalues, relation (34) is not sufficient to guarantee the series to be truncated. For this, we need to impose other conditions relating some other coefficients in the series. More precisely, for each \bar{n} , there are $\bar{n} + 1$ equations involving the coefficients $(C_0, \dots, C_{\bar{n}+3})$, with C_0 , C_1 and C_2 satisfying the following relations:

$$k_1 C_1 + (k_3 + k_5) C_0 = 0 \tag{37}$$

and

$$(3 + 2k_1) C_2 + (-1 + k_1 + k_3 + k_5) C_1 + (k_4 + k_5) C_0 = 0. \tag{38}$$

All these impositions lead to an expression involving a restriction on values taken by B , and a dependence on indices \bar{n} and ν is introduced. Here, since we work with a very complicated recurrence relation, we study only the three first cases. For $\bar{n} = 0$, we have

$$(6 + 3k_1)C_3 + (2k_1 + k_3 + k_5)C_2 + (k_2 + k_4 + k_5)C_1 = 0. \quad (39)$$

In this case, it is required that all coefficients are zero, except of C_0 . Besides, we want to have only one relation. The choice $k_3 = -k_5$ yields, by (37), $C_1 = 0$, but it does not allow us to write the relation between C_2 and C_1 using (37) and (38), because it is proportional to $(k_3 + k_5)^{-1}$. Thus, rigorously we cannot have $C_2 = 0$. So, we take the choice $C_0 = 0$ and vanishing of the wave function for $\bar{n} = 0$. This means that state with $\bar{n} = 0$ does not exist here and the first energy eigenvalue must be obtained for $\bar{n} = 1$ in (35). Obviously it is possible to cancel C_2 in (38) by assuming $k_4 = -k_5$ as a second relation, but that implies a contradiction.

For $\bar{n} = 1$, the equations are

$$(6 + 3k_1)C_3 + (2k_1 + k_3 + k_5)C_2 + (k_2 + k_4 + k_5)C_1 = k_2C_0 \quad (40)$$

and

$$(12 + 4k_1)C_4 + (3 + 3k_1 + k_3 + k_5)C_3 + (2k_2 + k_4 + k_5)C_2 = 0. \quad (41)$$

In order to cancel all coefficients after C_0 and C_1 , considering the relations (37) and (38), we should manipulate these two equations carefully. Thus, we can write

$$C_2 = \frac{1}{3 + 2k_1} \left[(-1 + k_1 + k_3 + k_5) \frac{(k_3 + k_5)}{k_1} - (k_4 + k_5) \right] C_0 \quad (42)$$

and

$$C_3 = -\frac{(2k_1 + k_3 + k_5)}{6 + 3k_1} C_2 - \frac{1}{6 + 3k_1} \left[\frac{(k_2 + k_4 + k_5)(k_3 + k_5)}{k_1} + k_2 \right] C_0. \quad (43)$$

By vanishing the bracket terms, we obtain $C_2 = 0$ and $C_3 = 0$. Consequently, expression (41) gives $C_4 = 0$. In addition, the following expression is obtained:

$$(-1 + k_3 + k_5)k_2 = (k_3 - k_4)k_5, \quad (44)$$

from where we find the equation for $B_{1\nu}$

$$\begin{aligned} [2(\nu - \gamma) - 1]B_{1\nu} \pm \frac{2m(\nu - \gamma)}{e(\gamma - \nu + 1)} [m^2 + (\gamma - \nu + 1)eB_{1\nu}]^{1/2} \\ + \frac{2m^2(\nu - \gamma)}{e(\gamma - \nu + 1)} = 0. \end{aligned} \quad (45)$$

In particular, for $m \ll |E|$ we can find $B_{1\nu}$:

$$B_{1\nu} = \frac{2m^2(\nu - \gamma)}{e(\gamma - \nu + 1)[1 - 2(\nu - \gamma)]}, \quad m \ll |E|. \quad (46)$$

For $\bar{n} = 2$, the same procedure is employed. The equations are

$$(6 + 3k_1)C_3 + (2k_1 + k_3 + k_5)C_2 + (k_2 + k_4 + k_5)C_1 = 2k_2C_0, \quad (47)$$

$$(12 + 4k_1)C_4 + (3 + 3k_1 + k_3 + k_5)C_3 + (2k_2 + k_4 + k_5)C_2 = k_2C_1 \quad (48)$$

and

$$(20 + 5k_1)C_5 + (8 + 4k_1 + k_3 + k_5)C_4 + (3k_2 + k_4 + k_5)C_3 = 0. \quad (49)$$

In an analogous way, from (47) we can write an expression relating C_3 and C_0 , which can be inserted in (48). Canceling the appropriate terms, the coefficients C_3 , C_4 and C_5 will be automatically zero in the series and an equation for B is determined. We find

$$(k_3 + k_5)(k_5 - k_2)k_5 + 2k_2k_1k_5 = -(2k_1 + k_3 + k_5)(k_3 + k_5)k_2. \quad (50)$$

This relation produces a very large and dense equation for the field $B_{2\nu}$. We will not present it here. However, a great simplification is found when we consider the case where $m \ll |E|$. In this case, Eq. (50) gives

$$B_{2\nu} = -(m^2[(\nu - \gamma) + 2\alpha^2]) \left(e(\gamma - \nu + 2)[(\nu - \gamma) + 2\alpha^2] - e \left[(2\gamma + 1)\alpha^2 \frac{1}{4}(\nu - \gamma)\epsilon_1 + \frac{1}{2}\epsilon_1\alpha^2 \right] \right)^{-1}, \quad (51)$$

with $\epsilon_1 = 3\gamma + \nu + 2$.

As we can see, results show that the discrete values allowed for the magnetic field B are determined by the quantum numbers \bar{n} and j and by the conical topology of the system, characterized by the parameter n . For each state \bar{n} , the magnetic field exhibits a set of values controlled directly by the topological aspects of the system. Considering the expressions (46) and (51) obtained above, in order to illustrate how energy responds to the defect, we plot the eigenvalues $E_{\bar{n}=1}$ and $E_{\bar{n}=2}$ in terms of the topological parameter n . The typical behavior can be observed in Figs. 3a and 3b. We note that, for both graphics, the eigenvalues show a decreasing dependence on n , i.e., they become lower when the number of removed sectors increases.

5. Concluding remarks

In this work, we have investigated the general properties of bound states of a massive fermion in a graphene cone with subcritical Coulomb charge impurity localized at its apex which interacts with a uniform magnetic field. A continuum description has been employed. The topological defect has been inserted by a specific vector potential which can reproduce the conical topology. This method correctly simulates terms in the Dirac equation usually found by a general geometric approach. Coulomb and magnetic fields have been incorporated by the usual way.

We have solved the Dirac equation by using the Frobenius method and have obtained exactly the eigenvalues of energy for this dynamics. The eigenvalues are found to depend on the parameters γ and ν , which contain the parameter n , responsible for characterizing the topological defect, and the strength of the external Coulomb impurity α . Particularly, the effect of conical topology on the spectrum can be realized by the presence of an effective quantum number ν replacing the angular momentum j , what corresponds to a practical tool to characterize the conical background. The presence of impurity eliminates the infinite degeneracy associated with the region $\nu > 0$. For this range, each level \bar{n} has infinite states with the same energy corresponding to the infinite values of angular momentum; the strength α ensures that the parameter ν does not disappear in the spectrum and, hence, the degeneracy is broken. Furthermore, eigenvalues also exhibit a dependence on the particular values of magnetic field $B_{\bar{n}\nu}$ and the mass m . A direct relation between these terms is also observed. The presence of the mass encodes the way by which the sublattice symmetry is broken and indicates how it modifies the physical properties of the system. Thus, this relation demonstrates an explicit connection between the gap generated by breaking the sublattice symmetry and the sets of topologically controllable values of magnetic field. As a

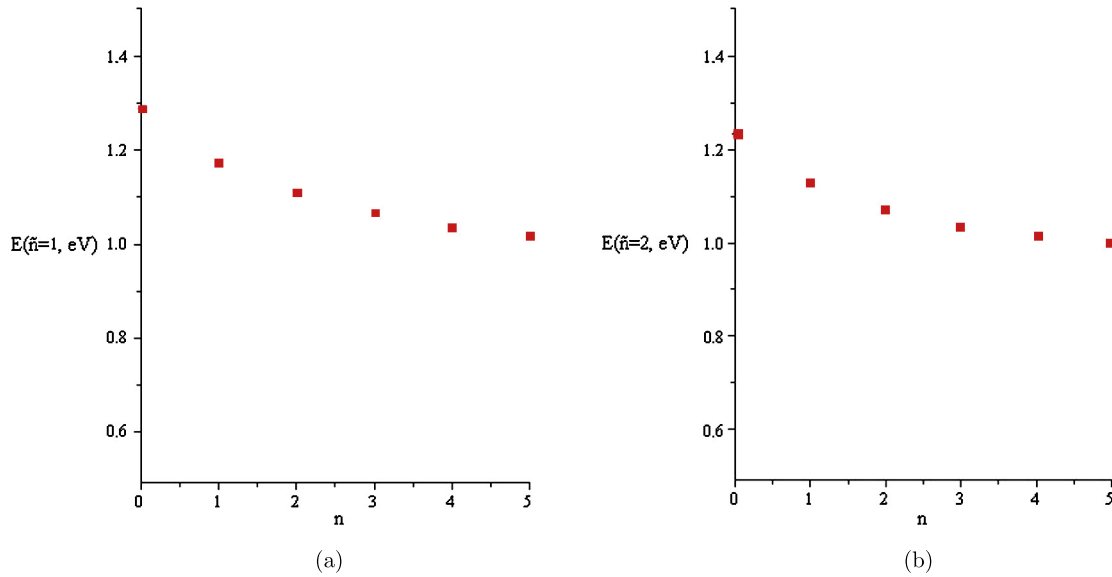


Fig. 3. (a) Plot of the eigenvalue $E_{\tilde{n}=1}$ in function of the parameter n , with $m = 1.0$, $e = 1.0$, $j = \frac{3}{2}$ and $\alpha = 0.75$. (b) Plot of the eigenvalue $E_{\tilde{n}=2}$ for the same values.

consequence, in addition to the explicit massive term in its expression, energy also responds to this asymmetry via magnetic field.

Some important results are obtained in the appropriate limits. In the limit $n = 0$, we recover the results obtained by Ho and Khalilov [58] for the relativistic quantum dynamics of an electron in the presence of Coulomb and strong magnetic fields. In the limiting case where we do not consider the Coulomb field of the impurity, i.e., for $\alpha = 0$, we restore the results for Landau levels in the presence of disclination in graphene layer [15,38]. This limit is obtained by making the limit $\alpha \rightarrow 0$ in Eq. (30); we cannot achieve this limit in subsequent equations due to the fact that the change of variable $u = (\frac{m+E}{\alpha})r$ blows up in this case.

It is important to point out that bound states cannot exist for any value of magnetic field. They only exist for sets of values obtained from the relations which make the solutions (32) to be normalizable. For each energy level, these discrete values are controlled by the topological parameter of the system, representing a relevant interference of topology on general physical aspects of the problem. Taking into account this fact, the graphics for $E_{\tilde{n}=1}$ and $E_{\tilde{n}=2}$ suggest that energies decrease when the number of removed sector increases. Similar situations where the eigenvalues and eigenfunctions are obtained not for any, but only for certain values of magnetic field, were observed for solutions of the Schrödinger equation yielding Landau levels in the presence of disclinations [59] and within the quantum dynamics of two anyons in the presence of a magnetic field [60]. Finally, we claim that the results obtained here can be utilized in future analytical investigations on the spectra of hydrogenic impurities in magnetic quantum dots of graphene [61] with topological defects.

Acknowledgements

This work was partially supported by CNPq (308788/2013-3) FAPESQ and CAPES, Brazilian agencies, and CAPES/NANOBIOTEC-99/2009. C.A.L.R. would like to thank MCT-CNPq for the support No. 565745/2008-5.

References

[1] S. Iijima, *Nature* 354 (1991) 56.
 [2] A. Krishnan, et al., *Nature* 388 (1997) 451.
 [3] L.D. Landau, E.M. Lifshitz, *Phys. Z. Sowjetunion* 11 (1937) 26.
 [4] N.D. Mermin, *Phys. Rev.* 176 (1968) 250.

[5] J.A. Venable, et al., *Rep. Prog. Phys.* 47 (1984) 399.
 [6] K.S. Novoselov, A.K. Geim, S.V. Morozov, D. Jiang, Y. Zhang, S.V. Dubonos, I.V. Grigorieva, A.A. Firsov, *Science* 306 (2004) 666.
 [7] P.E. Lammert, V.H. Crespi, *Phys. Rev. Lett.* 85 (2000) 5190.
 [8] R. Tamura, M. Tsukada, *Phys. Rev. B* 49 (1994) 7697.
 [9] S.Y. Zhou, G.-H. Gweon, A.V. Fedorov, P.N. First, W.A. de Herr, D.-H. Lee, F. Guinea, A.H. Castro Neto, A. Lanzara, *Nat. Mater.* 6 (2007) 770.
 [10] J. González, F. Guinea, M.A.H. Vozmediano, *Phys. Rev. Lett.* 69 (1992) 172.
 [11] J. González, F. Guinea, M.A.H. Vozmediano, *Nucl. Phys. B* 406 (1993) 771.
 [12] V.A. Osipov, E.A. Kochetov, *JETP Lett.* 73 (2001) 562.
 [13] V.A. Osipov, E.A. Kochetov, *JETP Lett.* 72 (2000) 199.
 [14] V.A. Osipov, E.A. Kochetov, M. Pudlak, *JETP Lett.* 96 (2003) 140.
 [15] P.E. Lammert, V.H. Crespi, *Phys. Rev. B* 69 (2004) 035406.
 [16] A. Cortijo, M.A.H. Vozmediano, *Nucl. Phys. B* 763 (2007) 293.
 [17] A. Cortijo, M.A.H. Vozmediano, *Europhys. Lett.* 77 (2007) 47002.
 [18] A. Cortijo, M.A.H. Vozmediano, *Eur. Phys. J. Spec. Top.* 148 (2007) 83.
 [19] P.R. Wallace, *Phys. Rev.* 71 (1947) 9.
 [20] D.P. Di Vincenzo, E.J. Mele, *Phys. Rev. B* 29 (1984) 1685.
 [21] C. Furtado, F. Moraes, A.M. de M. Carvalho, *Phys. Lett. A* 372 (2008) 5368.
 [22] K. Bakke, C. Furtado, S. Sergeenkov, *Europhys. Lett.* 87 (2009) 30002.
 [23] K. Bakke, A.Y. Petrov, C. Furtado, *Ann. Phys. (NY)* 327 (2012) 2946.
 [24] A.M. de M. Carvalho, C.A. de Lima Ribeiro, F. Moraes, C. Furtado, *Europhys. J. Plus* 128 (2013) 6.
 [25] M.A.H. Vozmediano, M.I. Katsnelson, F. Guinea, *Phys. Rep.* 496 (2010) 109.
 [26] K.S. Novoselov, A.K. Geim, S.V. Morozov, D. Jiang, Y. Zhang, S.V. Dubonos, I.V. Grigorieva, A.A. Firsov, *Nature* 438 (2005) 197.
 [27] T. Ando, *J. Phys. Soc. Jpn.* 75 (2006) 7.
 [28] E.H. Hwang, S. Adam, S. das Sarma, *Phys. Rev. Lett.* 98 (2007) 186806.
 [29] B. Chakraborty, K.S. Gupta, S. Sen, *Phys. Rev. B* 83 (2011) 115412.
 [30] B. Chakraborty, K.S. Gupta, S. Sen, *J. Phys. A, Math. Theor.* 46 (2013) 055303.
 [31] V.M. Pereira, J. Nilsson, A.H. Castro Neto, *Phys. Rev. Lett.* 99 (2007) 166802.
 [32] D.S. Novikov, *Phys. Rev. B* 76 (2007) 245435.
 [33] A.V. Shytov, M.I. Katsnelson, L.S. Levitov, *Phys. Rev. Lett.* 99 (2007) 246802.
 [34] V.M. Pereira, V.N. Kotov, A.H. Castro Neto, *Phys. Rev. B* 78 (2008) 085101.
 [35] K.S. Gupta, S. Sen, *Mod. Phys. Lett.* 24 (2009) 99.
 [36] B.S. Kandemir, A. Mogulkoc, *Eur. Phys. J. B* 74 (2010) 535.
 [37] J.L. Zhu, S. Sun, N. Yang, *Phys. Rev. B* 85 (2012) 035429.
 [38] M.J. Bueno, C. Furtado, A.M. de M. Carvalho, *Eur. Phys. J. B* 85 (2012) 53.
 [39] E.V. Gorbar, V.P. Gusynin, V.A. Miransky, I.A. Shovkovy, *Phys. Rev. B* 66 (2002) 045108.
 [40] D.V. Khveshchenko, H. Leal, *Nucl. Phys. B* 687 (2004) 323.
 [41] C.L. Kane, E.J. Mele, *Phys. Rev. Lett.* 95 (2005) 226801.
 [42] V.P. Gusynin, V.A. Miransky, S.G. Sharapov, I.A. Shovkovy, *Phys. Rev. B* 77 (2008) 205409.
 [43] D.V. Khveshchenko, *J. Phys. Condens. Matter* 21 (2009) 075303.
 [44] O.V. Gamayun, E.V. Gorbar, V.P. Gusynin, *Phys. Rev. B* 81 (2010) 075429.
 [45] W. Li, G.-Z. Liu, *Phys. Lett. A* 374 (2010) 2957.
 [46] Y. Araki, T. Hatsuda, *Phys. Rev. B* 82 (2010) 121403.
 [47] Y. Araki, *J. Phys. Conf. Ser.* 302 (2011) 012022.
 [48] M.Y. Han, et al., *Phys. Rev. Lett.* 98 (2007) 206805.
 [49] S.Y. Zhou, et al., *Nat. Mater.* 6 (2007) 770.
 [50] S.Y. Zhou, et al., *Nat. Mater.* 7 (2008) 259.

- [51] D. Haberer, et al., *Nano Lett.* 10 (2010) 3360.
- [52] D.R. Cooper, et al., *ISRN Condens. Matter Phys.* 2012 (2012) 501686.
- [53] E.Y. Andrei, et al., *Rep. Prog. Phys.* 75 (2012) 056501.
- [54] D.-K. Ki, A.F. Morpurgo, *Phys. Rev. Lett.* 108 (2012) 266601.
- [55] A.H. Castro-Neto, F. Guinea, N.M.R. Peres, K.S. Novoselov, A.K. Geim, *Rev. Mod. Phys.* 81 (2009) 109.
- [56] A.H. Castro-Neto, arXiv:1004.3682v1, 2010.
- [57] F. Moraes, *Braz. J. Phys.* 30 (2000) 2.
- [58] C.-L. Ho, V.R. Khalilov, *Phys. Rev. A* 61 (2000) 032104.
- [59] C. Furtado, et al., *Phys. Lett. A* 195 (1994) 90.
- [60] A. Verçin, *Phys. Lett. B* 260 (1991) 120.
- [61] C. Liu, J.-L. Zhu, N. Yang, *J. Appl. Phys.* 113 (2013) 224303.