Graphene physics via the Dirac oscillator in (2+1) dimensions

C. Quimbay[a†]

Departamento de Física, Universidad Nacional de Colombia.

Ciudad Universitaria, Bogotá D.C., Colombia.

P. Strange[‡]

School of Physical Science, University of Kent.

Canterbury, United Kingdom

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Abstract

We show how the two-dimensional Dirac oscillator model can describe some properties of electrons in graphene. This model explains the origin of the left-handed chirality observed for charge carriers in monolayer and bilayer graphene. The relativistic dispersion relation observed for monolayer graphene is obtained directly from the energy spectrum, while the parabolic dispersion relation observed for the case of bilayer graphene is obtained in the non-relativistic limit. Additionally, if an external magnetic field is applied, the unusual Landau-level spectrum for monolayer graphene is obtained, but for bilayer graphene the model predicts the existence of a magnetic field-dependent gap. Finally, this model also leads to the existence of a chiral phase transition.

Keywords: Dirac oscillator in (2+1) dimensions, electronic properties of graphene, monolayer and bilayer graphene, dispersion relations, Landau levels.

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[a] Associate researcher of Centro Internacional de Física, Bogotá D.C., Colombia.

[†] cjquimbayh@unal.edu.co

[‡] P.Strange@kent.ac.uk

The three-dimensional system defined by the Dirac equation in the presence of a linear vector potential of the form: $im\omega\beta\vec{\alpha}\cdot\vec{r}$, where m is the fermion mass, ω an oscillator frequency, $\vec{r}$ the vector distance of the fermion from the origin of the potential, and $\vec{\alpha}$ and β are the four Dirac matrices, has been called the Dirac oscillator [1] because it behaves in the non-relativistic limit as an harmonic oscillator with a strong spin-orbit coupling [2]. Different physics and mathematical aspects of this system have been widely studied in one, two and three dimensions [3]-[24]. Additionally, this system has been used in quantum optics to study properties of the (Anti)-Jaynes-Cummings model [25]-[31]. After more than 20 years of theoretical activity focussed in the characterization of the Dirac oscillator, just recently a first experimental realization of this system was developed [32]. However, until now the Dirac oscillator does not describe a known physical system [32].

On the other hand, the study of the electronic properties for monolayer and bilayer graphene has been of huge interest in recent years (see, for instance,[33–35] and references therein). It has been observed that electric charge carriers of monolayer graphene behave like massless relativistic fermions that obey a linear dispersion relation [33, 34], while the electric charge carriers for the case of bilayer graphene behave like massive non-relativistic fermions that obey a quadratic dispersion relation [34, 35]. For both systems, the explanation of the origin of these dispersion relations comes from the traditional tight-binding approach. However, the tight-binding Hamiltonians for electrons considering that electrons can hope to both nearest- and next-nearest-neighbor are different for both systems [33–35], thus this approach leads to different explanations of the origin of the distinct dispersion relations are of the two systems. In addition to the different behaviour of the energy spectra, it is difficult to understand how the massive electric charge carriers have a defined left-handed chirality for the case of bilayer graphene.

The main goal of this letter is to show for the first time that the Dirac oscillator can describe a naturally occurring physical system. Specifically, this work shows that the (2+1)-dimensional Dirac oscillator can be used to describe the dynamics of the charge carriers in graphene, and hence its electronic properties. To do this, we propose a model in which the electromagnetic interaction of the medium over charge carriers of graphene is described by means of a linear vector potential in the Dirac equation. Solution of the model shows that the same formalism can describe the linear relativistic dispersion relation for massless charge carriers of monolayer graphene and the parabolic dispersion relation for massive

charge carriers of bilayer graphene. The linear term that appears in the Dirac oscillator model leads directly to the left-handed chirality observed in the charge carriers for both monolayer and bilayer graphene. We also show that if an external and uniform magnetic field is present in the system, the model describes the unusual Landau levels observed for the case of monolayer graphene, while for bilayer graphene it predicts the existence of a magnetic field-dependent gap. Finally, we show that this model predicts that changing the strength of the magnetic field must lead to the existence of a chiral quantum phase transition for the system.

We propose a Dirac oscillator in (2+1) dimensions for which the linear potential has the form: $ieB_I\sigma_z\vec{\sigma}\cdot\vec{r}/4$, where $\vec{r}=(x,y)$, $\alpha_x=\sigma_x$, $\alpha_y=\sigma_y$, $\beta=\sigma_z$, e is the electrical charge of electron and B_I is an internal uniform effective magnetic field which is perpendicular to the plane ($\vec{B}_I=B_I\hat{e}_z$) and is assumed to originate in an effective form from the motion of the charge carriers relative to the planar hexagonal arrangement of carbon atoms. The model is based on the premise that the dynamics of charge carriers in graphene can be effectively described via this two-dimensional Dirac oscillator

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

where v_f is the Fermi speed of the charge carriers, m is the effective mass, p_j are the components of the linear momentum, r_j are the spatial coordinates in the (x,y) plane with respect to the origin of the potential, σ_j are the non-diagonal Pauli matrices, σ_z is the diagonal Pauli matrix. The assumption about the origin of B_I can be understood in analogous way to the internal magnetic field that determines the spin-orbit coupling of the hydrogen atom, which arises from the relative motion of the electron relative to the proton. It is well known that for the case of monolayer graphene in a perpendicular magnetic field [33], the Hamiltonian $H_{ml}=v_f[\tau\sigma_x(p_x-ieB_I\sigma_z x/4)+\sigma_y(p_y-ieB_I\sigma_z y/4)]$ describes the single-particle states around one of the two equivalent corners of the first Brillouin zone. $\tau=\pm1$ determines which corner of the Brillouin zone is considered [36]. This fact means that we are considering in Eq. (1) the corner defined by $\tau=1$.

For the case of monolayer graphene, the charge carriers are considered massless ($m=0$) and the mass term in Eq. (1) does not exist. The spinor $\mid\psi>$ is written as $\mid\psi>=(\mid\psi_1>,\mid$

$\psi_2 >)^T$. Substituting this spinor in Eq. (1), we obtain the following two coupled equations

$$(E - mv_f^2) \mid \psi_1 > = v_f \left[(p_x + i\frac{\hbar\omega^2}{v_f^2}x) - i(p_y + i\frac{\hbar\omega^2}{v_f^2}y) \right] \mid \psi_2 >, \tag{2}$$

$$(E + mv_f^2) \mid \psi_2 > = v_f \left[(p_x - i\frac{\hbar\omega^2}{v_f^2}x) + i(p_y - i\frac{\hbar\omega^2}{v_f^2}y) \right] \mid \psi_1 >, \tag{3}$$

where $\omega^2 = v_f^2/(4l_B^2)$, with $l_B^2 = \hbar/(eB_I)$. The quantity l_B represents a new length scale in the problem associated to the quantity eB_I that appears in the linear potential. In order to find the solutions of Eqs. (2) and (3), we introduce the right-handed chiral annihilation and creation operators given by $a_r = \frac{1}{\sqrt{2}}(a_x - ia_y)$, $a_r^\dagger = \frac{1}{\sqrt{2}}(a_x^\dagger + ia_y^\dagger)$ and the left-handed chiral annihilation and creation operators given by $a_l = \frac{1}{\sqrt{2}}(a_x + ia_y)$, $a_l^\dagger = \frac{1}{\sqrt{2}}(a_x^\dagger - ia_y^\dagger)$, where a_x, a_y, $a_x^\dagger$ and $a_y^\dagger$ are the usual annihilation and creation operators of the harmonic oscillator defined respectively as $a_j = \frac{1}{\sqrt{2}}\left(\frac{1}{\Delta}r_j + i\frac{\Delta}{\hbar}p_j\right)$ and $a_j^\dagger = \frac{1}{\sqrt{2}}\left(\frac{1}{\Delta}r_j - i\frac{\Delta}{\hbar}p_j\right)$, with $\Delta = v_f/\omega$ representing the ground-state oscillator width. Because the orbital angular momentum L_z is written in terms of the chiral annihilation and creation operators as $L_z = \hbar(a_r^\dagger a_r - a_l^\dagger a_l)$, then $a_r^\dagger$ and $a_l^\dagger$ are interpreted as the operators that create a right or left quantum of angular momentum, respectively [25]. After expressing r_j and p_j in terms of operators a_j and $a_j^\dagger$, the Eqs. (2) and (3) lead to

$$\mid \psi_1 > = i\frac{2\hbar\omega}{E - mv_f^2}a_l^\dagger \mid \psi_2 >, \tag{4}$$

$$\mid \psi_2 > = -i\frac{2\hbar\omega}{E + mv_f^2}a_l \mid \psi_1 >, \tag{5}$$

where only the left-handed chiral operators are present [25]. If we substitute Eqs. (4) and (5) in (1), the Hamiltonian describing the dynamics of charge carriers in graphene can be written as

$$H_1 = \hbar(g_l\sigma^+ a_l^\dagger + g_l^*\sigma^- a_l) + mv_f^2\sigma_z, \tag{6}$$

with σ^+ and σ^- representing the spin raising and lowering operators and $g_l = i2\omega = iv_f\sqrt{eB_I/\hbar}$. The two-dimensional Hamiltonian H_1 describes a massive charge carrier of left-handed chirality.

From Eqs. (4) and (5), it is possible to write the associated Klein-Gordon equations and then to obtain the energy spectrum for charge carriers of left-handed chirality

$$E_{n_l} = \pm\sqrt{\hbar^2k^2v_f^2\left(n_l + \frac{1}{2} \mp \frac{1}{2}\right) + m^2v_f^4}, \tag{7}$$

with $n_l = 0, 1, 2, \ldots$ and $k^2 = eB_I/\hbar$. For the case in which the effective mass of charge carriers vanishes ($m = 0$), the energy spectrum (7) is written as

$$E_{n_l} = \pm\hbar k v_f \sqrt{n_l + \frac{1}{2} \mp \frac{1}{2}}, \tag{8}$$

which corresponds to the relativistic dispersion relation depending linearly on the momentum $\hbar k$ and which is consistent with the well known result for charge carriers in monolayer graphene [33, 34]. On the other hand, for the case where the effective mass of the charge carriers is non-zero ($m \neq 0$), the non-relativistic limit of (7) yields

$$E^{nr}_{n_l} = \pm\sqrt{\hbar^2 k^2 v_f^2 \left(n_l + \frac{1}{2} \mp \frac{1}{2}\right) + m^2 v_f^4} - m v_f^2. \tag{9}$$

For this limit, it is valid to write $mv_f \gg \hbar k$ and then the energy spectrum for charge carriers can be written as

$$E^{+}_{n_l} = \frac{\hbar^2 k^2}{2m}\left(n_l + \frac{1}{2} \mp \frac{1}{2}\right), \tag{10}$$

which corresponds to the non-relativistic dispersion relation depending parabolically on the momentum, which is observed for charge carriers in bilayer graphene [37]. We note that, within the same theoretical formalism, we have been able to obtain the very well known dispersion relations of charge carriers in monolayer and bilayer graphene, that are usually obtained starting from the standard nearest-neighbour approximation using two different tight-binding Hamiltonians [33–35]. Because the linear term of the Dirac oscillator leads directly to a description of a fermion with an intrinsic left-handed chirality, which is only present in the two-dimensional Dirac oscillator [25], the charge carriers of graphene describe by Eq. (1) are left-handed. In this sense, the Dirac oscillator described by equation (1) can explain the left-handed chirality observe for massless and massive charge carriers in graphene.

Next we consider the effect of an external uniform magnetic field on the system. The dynamics of the charge carriers of graphene are then described by

$$i\hbar\frac{\partial}{\partial t} \mid \psi >= \left[v_f \sum_{i=1}^{2} \sigma_j \left(p_j - i\frac{eB_I}{4}\sigma_z r_j - eA_j\right) + \sigma_z m v_f^2\right] \mid \psi >, \tag{11}$$

where we are considering the corner of the first Brillouin zone defined by $\tau = 1$ [36]. We observe that for the case of a vanishing magnetic field ($A_j = 0$) in Eq. (11), then the Eq. (1)

is recovered. In order to understand the physics described by Eq. (11), we assume initially that the linear potential in vanishes. This fact means we are considering an charge carriers with mass in presence of an external magnetic field. i.e.

$$i\hbar\frac{\partial}{\partial t} \mid \psi >= \left[v_f \sum_{i=1}^{2} \sigma_j \left(p_j - eA_j \right) + \sigma_z m v_f^2 \right] \mid \psi > . \tag{12}$$

Substituting the spinor $\mid \psi >= (\mid \psi_1 >, \mid \psi_2 >)^T$ in Eq. (12), yields following two coupling equations:

$$(E - mv_f^2) \mid \psi_1 > = v_f[(p_x - eA_x) - i(p_y - eA_y)] \mid \psi_2 >, \tag{13}$$

$$(E + mv_f^2) \mid \psi_2 > = v_f[(p_x - eA_x) + i(p_y - eA_y)] \mid \psi_1 >, \tag{14}$$

The external magnetic field, which is perpendicular to the plane, is written as $\vec{B} = -B\hat{e}_z$. The vector potential $\vec{A}$ then has the form $\vec{A} = (A_x, A_y, A_z) = \frac{B}{2}(y, -x, 0)$. With this vector potential, Eqs. (13) and (14) become

$$(E - mv_f^2) \mid \psi_1 > = v_f[(p_x - i\frac{\hbar\tilde{\omega}^2}{v_f^2}x) - i(p_y - i\frac{\hbar\tilde{\omega}^2}{v_f^2}y)] \mid \psi_2 >, \tag{15}$$

$$(E + mv_f^2) \mid \psi_1 > = v_f[(p_x + i\frac{\hbar\tilde{\omega}^2}{v_f^2}x) + i(p_y + i\frac{\hbar\tilde{\omega}^2}{v_f^2}y)] \mid \psi_2 >, \tag{16}$$

where $\tilde{\omega}^2 = \omega_c^2/2$, with the cyclotron frequency ω_c defined by $\omega_c^2 = eBv_f^2/\hbar$. To solve Eqs. (15) and (16), we again introduce the right- and left-handed chiral annihilation and creation operators [26]. Then we write r_j and p_j in terms of operators $\tilde{a}_j$ and $\tilde{a}_j^\dagger$, from Eqs. (15) and (16) we obtain

$$\mid \psi_1 > = -i\frac{2\hbar\tilde{\omega}}{E - mv_f^2}\tilde{a}_r \mid \psi_2 >, \tag{17}$$

$$\mid \psi_2 > = i\frac{2\hbar\tilde{\omega}}{E + mv_f^2}\tilde{a}_r^\dagger \mid \psi_1 > . \tag{18}$$

In contrast to Eqs. (4) and (5), where only the left-handed chiral operators appear, here in Eqs. (17) and (18) only the right-handed chiral operators are present[26]. Substituting Eqs. (17) and (18) into Eq. (12), it is possible to write the Hamiltonian of this system in the following form

$$H_2 = -\hbar(\tilde{g}_r\sigma^+\tilde{a}_r + \tilde{g}_r^*\sigma^-\tilde{a}_r^\dagger) + mv_f^2\sigma_z, \tag{19}$$

with $\tilde{g}_r = 2i\tilde{\omega} = iv_f\sqrt{2eB/\hbar}$. The Hamiltonian H_2 describes a massive electron of right-handed chirality. From Eqs. (17) and (18), we obtain the energy spectrum given by

$$E_{n_r} = \pm\sqrt{2eB\hbar v_f^2\left(n_r + \frac{1}{2} \pm \frac{1}{2}\right) + m^2v_f^4}, \tag{20}$$

with $n_r = 0, 1, 2, \ldots$. For the case of massless charge carriers the energy spectrum (20) is written as

$$E_{n_r} = \pm\sqrt{2eB\hbar v_f^2\left(n_r + \frac{1}{2} \pm \frac{1}{2}\right)}, \tag{21}$$

which corresponds to the well-known unusual Landau-level spectrum of monolayer graphene [38–40]. We note that the expression (21) has exactly the same form as the Landau levels given by expression (1) of the reference [41]. On the other hand, for the case $m \neq 0$, the non-relativistic limit of (20) leads to the following result

$$E_{n_r}^{n-r} = \pm\sqrt{2eB\hbar v_f^2\left(n_r + \frac{1}{2} \pm \frac{1}{2}\right) + m^2v_f^4} - mv_f^2, \tag{22}$$

which corresponds to the Landau levels for bilayer graphene. This Landau-level spectrum implies that one of the levels obtained for $n_r = 0$ has a B-dependent gap of the form

$$\Delta E_0^{n-r} = -\delta + \sqrt{\gamma B + \delta^2}, \tag{23}$$

where $\delta = 2mv_f^2$ and $\gamma = 8ev_f^2\hbar$. This result has certain analogy with the experimental gap reported in [42]. The non-relativistic limit of (20) implies that $\delta^2 \gg \gamma B$, thus the Landau levels can be written as $E_{n_r}^{n-r} = eB/\hbar(n_r + \frac{1}{2} \pm \frac{1}{2})$ and the B-dependent gap obtained for one of the levels associated to $n_r = 0$ is written as $\Delta E_0^{n-r} = 2eB\hbar/m$. We note that the charge carriers described by Eq. (12) have right-handed chirality.

For the full problem described by Eq. (11), we consider simultaneously the two systems described by Hamiltonians (6) and (19). The Hamiltonian that describes the dynamics of charge carriers of graphene in presence of a uniform magnetic field is given by

$$H = H_l - H_r + mv_f^2\sigma_z, \tag{24}$$

where the left-handed Hamiltonian H_l is given by

$$H_l = \hbar(g_l\sigma^+a_l^\dagger + g_l^*\sigma^-a_l), \tag{25}$$

with $g_l = iv_f\sqrt{eB_I/\hbar}$, and the right-handed Hamiltonian H_r is given by

$$H_r = \hbar(\tilde{g}_r\sigma^+\tilde{a}_r + \tilde{g}_r^*\sigma^-\tilde{a}_r^\dagger), \tag{26}$$

with $\tilde{g}_r = iv_f\sqrt{2eB/\hbar}$.

For the case of a weak external field $B \ll B_I$, in a first approximation where corrections of order $O(B/B_I)$ are neglected, Eq. (11) leads to the energy spectrum given by (7). On the other hand, for the case of a strong external magnetic field $B \gg B_I$, neglecting corrections of order $O(B_I/B)$, the Eq. (11) leads to the energy spectrum of (20). This means that in the limit $B \to 0$ the charge carriers have left-handed chirality, while for the limit $B \to \infty$ they have right-handed chirality. In other words, changing the strength of the external magnetic field B must lead to the existence of a chiral quantum phase transition for the system described by Eq. (11). A complete characterization of this kind of chiral phase transition, using the two-dimensional Dirac oscillator couplings in the context of (Anti) Jaynes-Cummings models, is performed in reference [28] and the signatures of a possible quantum phase transition for the case of a graphene quantum dot model in a magnetic field has been reported in [43].

Without considering the presence of the external magnetic field, for the case of massless charge carriers (monolayer graphene), the left-handed hamiltonian is given by (26), while for the case of massive charge carriers (bilayer graphene), the left-handed hamiltonian is given by (6). Both these Hamiltonians can be described within a tight-binding model as shown in [32], for the one-dimensional Dirac oscillator. This fact means that the Dirac oscillator description, that we have introduced in this work, is consistent with the tight-binding approximation that traditionally has been used to describe the electronic structure of graphene [38–40].

The results that we have presented in this letter have shown that the two-dimensional Dirac oscillator describes consistently some electronic properties of graphene. This is the first time that the Dirac oscillator describes a very well know physics system. With the present model, it has been possible to explain that the left-handed chirality of charge carriers in monolayer and bilayer graphene is originated by the linear potential that appears in the Dirac oscillator model. This linear potential describes the interactions of the medium over the charge carriers. We have interpreted the parameter B_I that appears in the linear potential as an internal field acting over the charge carriers, which is assumed to originate in an effective

form from the motion of the charge carriers relative to the planar hexagonal arrangement of carbon atoms. This model leads consistently to the very well known dispersion relations of charge carriers in monolayer and bilayer graphene which traditionally are obtained using a tight-binding approximation. For the case in which an external and uniform magnetic field B is presented in a perpedicular form over the layers, the well known Landau level spectrum for the monolayer graphene is obtained. For the case of bilayer graphene, the model predicts the existence of a B-dependent gap. Finally, this model also predicts that changing the strength of B must lead to the existence of a chiral quantum phase transition for the system.

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