Energy spectrum for charge carriers in graphene with folded deformations or uniaxial flexural modes: analogies to the quantum Hall effect under random pseudo-magnetic fields.

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(Dated: 10 August 2021)

The electronic behaviour in graphene under arbitrary uniaxial deformations, such as foldings or flexural fields is studied by including in the Dirac equation pseudo-electromagnetic fields. General foldings are thus studied by showing that uniaxial deformations can be considered as pseudo-magnetic fields in the Coulomb gauge norm. This allows to give an expression for the Fermi (zero) energy modes wavefunctions. For random deformations, contact is made with previous works on the quantum Hall effect under random magnetic fields, showing that the density of states has a power law behaviour and that the zero energy modes wavefunctions are multifractal. This hints of an unusual electron velocity distribution. Also, it is shown that a strong Aharonov-Bohm pseudo-effect is produced. For more general non-uniaxial general flexural strain, it is not possible to use the Coulomb gauge. The results presented here allow to tailor-made graphene uniaxial deformations to achieve specific wave-functions and electronic properties.

I. INTRODUCTION

Recently, Dirac materials have attracted intense research interest following the celebrated discovery of a two-dimensional (2D) hexagonal allotropic atomic carbon, graphene, because of its peculiar band structure and its fascinating properties largely due to the massless Dirac fermion behavior of the charge carriers.

Due to such excellent mechanical, magnetic and thermal properties of graphite monolayers, they can be used for the development of superconducting devices for micro-electromechanical and nano-electromechanical systems, leading to the development of the next generation of nanoelectronics. As the use of graphene sheets increases, the understanding of the mechanical behaviour is necessary and important for the design and analysis of graphene nanostructures and nanosystems. This opened a new field of research known as straintronics, which aims to refine nanostructures and nanosystems. This opened a new field of research known as straintronics, which aims to refine nanoelectronic devices in the direction parallel to the fold axis, providing a normally flat substrate can be forced to undergo a buckling transition, resulting in a periodically modulated pseudo-magnetic field, which in turn creates a 'post-graphene' material with flat electronic bands. This buckling of 2D crystals offers a strategy for exploring interaction phenomena characteristic of flat bands.

In addition, there is an growing interest in folded deformations due to transport properties of strained folds in graphene exhibit a rich behavior ranging from Coulomb blockade to Fabry-Pérot oscillations for different fold orientations. Those exhibiting strong confinement, behave as electronic waveguides in the direction parallel to the fold axis, providing a new way to realize 1D conducting channels in 2D graphene by strain engineering. In general, the mechanical displacements on graphene causes strong changes in the vacuum-induced shifts of the transition frequency of some emitter and, because its low mass and high $Q$ factor, make it a particular attractive candidate for a wide class of sensors.

Most previous work concerning this topic has been focused in studying the electron mobility thorough using transport equations. In the present work, we study the effects on charge carriers due to the presence of pseudo-electromagnetic fields which models the case of vertical fluctuations due to folded deformations or flexural modes. These modes have...
a large phonon population originating from the quadratic phonon dispersion and are known to dominate the electron scattering\textsuperscript{31,33} and thermal transport\textsuperscript{33,34}. In particular, we show that for certain kind of flexural fields, one can make close contact with previous works on Dirac fermions in random electromagnetic potentials, besides its close relationship with the phase transition between the plateaus in Hall’s quantum states and the quasi-excitations in $d$-wave superconductors\textsuperscript{35}. Then we show that for more general fields, the Coulomb gauge condition used in this work can not be fulfilled.

It is important to remark that the methods presented here can be extended to study other optoelectronic properties in 2D materials, such as phosphorene or borophene, and these effects can also be studied using the present methodology, as plane deformations or flexural waves can be considered as random pseudo-electromagnetic waves; in addition, the present results can be extended for new Dirac materials\textsuperscript{37,38}.

The work is organized as follows. In Sec. III we introduce the effective Hamiltonian for low energies and obtain the time-independent Schrödinger equation to be solved. In Sec. IV we analyze specifically the electronic properties of graphene with folded deformations. And finally, we present the conclusions in Section V.

II. HAMILTONIAN MODEL

Out-of-plane acoustic modes are characteristic vibrations in graphene. These low frequency modes are easy to excite and carry most of the vibrational energy\textsuperscript{23,39}. They consist in a dynamic elongation, bending and torsion of the local bonds. The stretching or tension of the bonds is by far the most important for the electrons, since it causes a greater impact on the tunneling parameter\textsuperscript{4}. Some lattice deformations can be expressed by a gauge field using a Hamiltonian at low energies\textsuperscript{11,23}.

The low-energy Hamiltonian for non-interacting electrons in deformed graphene is a Dirac-type Hamiltonian and is given by\textsuperscript{14,23,40,41,42}

$$\hat{\mathcal{H}}_\eta(r) = v_F \eta \cdot (\hat{\mathbf{p}} - \eta \mathbf{A}(r,t)) + \mathbf{V}(r,t)\mathbb{I}_{2\times2},$$

where $\mathbf{r} = (x,y)$ is the position vector, the subscript $\eta = \pm 1$ labels the Dirac points $\mathbf{K}, \mathbf{K}'$ respectively; $v_F$ is the Fermi velocity ($v_F/c \approx 1/300$ with $c$ is the vacuum speed of light); $\hat{\mathbf{p}} = (\hat{p}_x,\hat{p}_y)$ is the momentum operator for the charge carriers, $\sigma = (\eta \sigma_x, \eta \sigma_y)$ is the Pauli matrix vector, and $\mathbf{A}$ and $\mathbf{V}$ are the pseudo vector and scalar potentials respectively, given by\textsuperscript{13,14,23}.

$$\mathbf{V}(r,t) = g(\varepsilon_{xx} + \varepsilon_{yy})$$

$$\mathbf{A}(r,t) = (A_x,A_y) = \frac{\hbar \beta}{2a_{cc}}(\varepsilon_{xx} - \varepsilon_{yy}, -2\varepsilon_{xy})$$

The parameter $g$ takes values from 0 to 20 eV\textsuperscript{11,41}, $a_{cc} = 1.42$ Å is the interatomic distance for undeformed graphene lattice, the dimensionless coefficient $\beta \approx 3.0$ measures the effect of the deformation on the hopping parameter. The coefficient $g$ refers to flexural changes in the membrane while the term $\hbar \beta/2a_{cc}$ refers to changes in bond length, as we know it requires more energy to make bond length changes to a rearrangement in the positions of the atoms on the membrane\textsuperscript{42}.

Therefore depending on how “strong” the deformations are we can vary the value of $g$ within a range of energies, while the factor $\hbar \beta/2a_{cc}$ remains approximately constant (within the validity range of our model).

In general, we can consider a displacement outside the plane $h = h(r,t)$, and a displacement inside the plane $\mathbf{u} = \mathbf{u}(r,t)$. The stress tensor $\varepsilon_{\mu\nu}$ is given by

$$\varepsilon_{\mu\nu} = \frac{1}{2} \left( \partial_\mu h \partial_\nu h + \frac{1}{2} \left( \partial_\mu u_\nu + \partial_\nu u_\mu \right) \right), \quad \mu, \nu = x, y.$$  

We shall consider the simplest case, in which the deformation is only perpendicular to the plane, i.e., $\mathbf{u} = 0$, so from Eq. 4

$$\varepsilon_{xx} = \frac{1}{2} (\partial_x h)^2$$

$$\varepsilon_{yy} = \frac{1}{2} (\partial_y h)^2$$

$$\varepsilon_{xy} = \frac{1}{2} (\partial_x h)(\partial_y h)$$

We introduce new variables defined as

$$l_1(r,t) = (\partial_x h)^2 - (\partial_y h)^2$$

$$l_2(r,t) = 2(\partial_x h)(\partial_y h)$$

which will give us information about how “strong” the vertical displacements are. On the other hand, by making use of the Eqs. 2, 3, 5 and 6, we can rewrite the scalar and pseudo-vector potentials,

$$\mathbf{V}(r,t) = \frac{g}{2} \sqrt{l_1(r,t)^2 + l_2(r,t)^2}$$

$$\mathbf{A}(r,t) = \frac{\hbar \beta}{4a_{cc}} (l_1(r,t)\hat{x} - l_2(r,t)\hat{y}).$$

From Eq. 1 and 7, the Hamiltonian is

$$\hat{\mathcal{H}}_\eta(r) = \hat{\mathcal{H}}_0(r) + \mathbf{W}(r,t) + \frac{g}{2} |l(r,t)| \mathbb{I}$$

where the hat is used to denote differential operators as follows,

$$\hat{\mathcal{H}}_0(r) = v_F \begin{pmatrix} 0 & (\eta \hat{\beta}_x - i \hat{\beta}_y) \\ (\eta \hat{\beta}_x + i \hat{\beta}_y) & 0 \end{pmatrix}$$

$$\mathbf{W}(r,t) = \begin{pmatrix} 0 & -\eta \hat{\beta}l(r,t) \\ -\eta \hat{\beta}l(r,t) & 0 \end{pmatrix}$$

where $l(r,t) \equiv \eta l_1(r,t) + il_2(r,t)$ and we defined the parameter $\hat{\beta}$ as,

$$\hat{\beta} = \frac{v_F \hbar \beta}{4a_{cc}} \approx 3.476471 \text{ eV}$$

The dynamic equation for the spinor $\Psi_\eta(r,t)$ follows a time-dependent Schrödinger type equation

$$i\hbar \frac{\partial}{\partial t} \Psi_\eta(r,t) = \hat{\mathcal{H}}_\eta(r) \Psi_\eta(r,t)$$
It is straightforward to prove that the Schrödinger type equation (11) can be rewritten as
\[
\frac{i\hbar}{2} \frac{\partial \Psi_A}{\partial t} = \frac{g}{2} [l | \Psi_A^n + [v_F (\eta \hat{p}_x - i \hat{p}_y) - \eta \hat{b} l] | \Psi_B^n].
\]
\[
\frac{i\hbar}{2} \frac{\partial \Psi_B}{\partial t} = \frac{g}{2} [l | \Psi_B^n + [v_F (\eta \hat{p}_x + i \hat{p}_y) - \eta \hat{b} l] | \Psi_A^n].
\]

Notice how the magnitude of the disorder enters in the argument
\[
\Psi_{\eta}(r, t) = \left( \begin{array}{c} \Psi_A^n(r, t) \\ \Psi_B^n(r, t) \end{array} \right).
\]

where
\[
A_i = \varepsilon_{ij} \partial_j \Phi(r)
\]

with, 
\[
\Phi(r) = \Phi_0(y) + \sum_{k \neq 0} e^{ik \hat{y}} \Phi(k)
\]

The associated pseudomagnetic field is 
\[
B = \nabla \Phi(r).
\]

III. FOLDED DEFORMATIONS

To understand the changes induced by random flexural deformations, we study folded deformations. Such kind of fields have been observed experimentally in deformed graphene and there are some studies for particular deformations. In a general folded deformation, the field does not vary in one direction. Therefore, it can be written as,
\[
h(y) = \sum_{k = -k_c}^{k_c} a_k \text{exp}(iky)
\]

with \(a_{-k} = a_k^*\) as \(h(y)\) is a real, and the coefficients \(a_k\) can be deterministic or random variables. \(k_c\) is a cutoff parameter and in what follows all sums are understood to use it. \(k_c\) can be estimated from the Bose-Einstein distribution and the frequency dispersion of flexural modes.

From Eqs. (3) and (4), the vectorial potential has only one component different from zero,
\[
A_y(y) = \frac{\hbar \beta}{4a_{cc}} \left[ \sum_k a_k \text{exp}(iky) \right]^2
\]

The advantage of this particular deformation is that \(A(r)\) is in the Coulomb gauge, as it satisfies \(\nabla \cdot A(r) = 0\), therefore it can be obtained as the derivative of a scalar field,
\[
\Phi(y) = \phi_0(y) + \sum_{k \neq 0} e^{ik \hat{y}} \Phi(k)
\]

with,
\[
\Phi_0(y) = \frac{\hbar \beta}{4a_{cc}} \left( \sum_k k^2 |a_k|^2 \right) y
\]

and,
\[
\Phi(k) = -i \frac{\hbar \beta}{4a_{cc}} \left[ \sum_{k'} a_k a_{k'}^* \delta(k' - k) \right]
\]

The associated pseudomagnetic field is 
\[
B = \nabla \Phi(r).
\]

An interesting consequence of having a field derived from the potential is that for any flexural field, being deterministic or random, the zero-mode can always be constructed. From the Schrödinger and Eq. (16), we obtain that for \(E = 0\) and \(g = 0\) the wave function is,
\[
\psi_\pm(r) = (\text{const.}) (1 \pm \sigma_z) \left( \frac{e^{i \phi(r)}}{e^{-i \phi(r)}} \right)
\]

where \(\sigma_z\) is the Pauli \(z\) matrix. Similar functions were studied years ago in the context of the integer quantum Hall transition. It can be proved that for a random magnetic field in which the vector potential satisfies a Gaussian white-noise distribution with mean zero and variance \(\Delta_A\) such that the average coefficients in Eq. (17) are,
\[
\langle \Phi(k) \Phi(k') \rangle = (2\pi)^2 (k - k') \frac{\Delta_A}{k^2}
\]

while the resulting wave-function is multifractal. In a sample of size \(L \times L\), the moments of the participation ratio \(P_q(L)\) that measures a multifractal localization,
\[
P_q(L) = \langle |\psi(r)|^{2q} \rangle
\]

are given by,
\[
P_q(L) \approx \frac{1}{L^{2+\tau(q)}}
\]

with,
\[
\tau(q) = 2(q - 1) + \frac{\Delta_A}{\pi} q(1 - q)
\]
where \( q \) need not be integer. For big samples, the multifractal spectrum is dominated by its maximal value, from where the typical participation is

\[
P_{\text{typical}}(L) = e^{\langle |\psi|^2 \rangle} \approx \frac{1}{L^{2+\Delta_A/\pi}} \quad (25)
\]

Around these states and near the Fermi energy, the density of states (DOS) is

\[
\rho(E) = E^{\frac{z}{2}} \quad (26)
\]

with \( z = 2 + \Delta_A/\pi \). Such wavefunction multifractality and DOS means that an unusual electron velocity distribution will appear even in the simplest case of a Gaussian random flexural field, without restoring to Levy distributions of membrane jumps in graphene. In any case, the Levy jumps will induce an even more unusual distributions.

We end up by considering the particular contribution of the Aharonov-Bohm term which for some geometries produces interesting effects in graphene, nevertheless has not been studied for random fields. First we write the Fourier coefficients \( d_k \) as the sum of an average plus a fluctuation part, \( d_k = \langle d_k \rangle + \delta d_k \). If \( a_k \) is Gaussian distributed with zero mean we have,

\[
\Phi_0(y) = \frac{\hbar B}{4a_{cc}} \sum_k (\delta d_k)^2 k^2 y \approx \frac{\pi \hbar B}{6 a_{cc}} \Delta_A k^3 y \quad (27)
\]

and thus the phase difference between particles, with the same start and end points, but travelling along two different paths is,

\[
\Delta \phi = \left( \frac{d \Phi_0(y)}{dy} \right)_{\partial \Omega} \frac{e}{\hbar} = \frac{\pi \beta}{6 a_{cc}} (\Delta_A k^3) e \quad (28)
\]

where \( \partial \Omega \) is the area bounded by the two paths. For thermally activated fields, \( k_c \) is determined from the temperature \( (T) \) population given by the Bose-Einstein distribution. As \( \Delta_A \sim k_B T \), Eq. \( (28) \) implies a very strong temperature dependent phase shift. This result is in agreement with recent first-principles calculations based on density functional theory and the Boltzmann equation.

### IV. CONCLUSIONS.

We studied the effects in the electronic properties of graphene of folded flexural deformations, which are equivalent to electromagnetic fields in the Coulomb gauge. First we studied general folded deformations giving an expression for the zero-modes which are the ones at the Fermi level for half-filled systems. For random Gaussian distributed folded deformations, we made contact with works on the quantum Hall effect under random magnetic fields, showing that the density of states has a power law behavior. This indicates that the system can present interesting behaviors. In particular, we showed that there is a remarkable Aharonov-Bohm pseudo-effect and wavefunction multifractality, which means that an unusual electron velocity distribution will appear even at this early stage of deformation.

### ACKNOWLEDGMENTS

We are grateful to Alejandro Pérez Riascos for their support and feedback in carrying out this work. We thank UNAM-DGAPA PAPIIT project IN102620 and CONACYT project 1564464. A.E.C. thanks CONACYT for providing a scholarship.

### DATA AVAILABILITY

The data that support the findings of this study are available from the corresponding author upon reasonable request.

### Appendix A

Although some works assume the Coulomb norm for general pseudo-electromagnetic fields, let us show that in general such deformation cannot be written as the derivative of a scalar field. This can be proved as follows, if we consider \( A_i(r) = e_{ij} \partial_j \Phi(r) \) with \( \Phi(r) = \sum_k b_k \exp(ik \cdot r) \) it holds that

\[
b_k = -\frac{i e \beta}{k_y} \sum_{k'} a_{k'} a_k^* (k_{i'} - k_{y'}) e^{-ik' \cdot r}
\]

and

\[
b_k = -\frac{i e \beta}{k_x} \sum_{k'} a_{k'} a_k^* (k_{x'} + k_{y'}) e^{-ik' \cdot r}
\]

In general, the system of equations in Eq. \( (A1) \) has no solutions for \( b_k \) except for few particular cases, as the folded potential studied here.

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