Induced fractional valley number in graphene with topological defects

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We report on the possibility of valley number fractionalization in graphene with a topological defect that is accounted for in the Dirac equation by a pseudomagnetic field. The valley number fractionalization is attributable to an imbalance in the number of one-particle states in one of the two Dirac points with respect to the other. The difference in the number of one-particle states is manifest and can be exactly evaluated thanks to an external uniform magnetic field. Although the external magnetic field is precluded, the net valley number results in being dependent only on the flux of the pseudomagnetic field. We also discuss the analogous effect that the topological defect might lead to the induced spin polarization of the charge carriers in graphene.

I. INTRODUCTION

Approximately seven years ago it was demonstrated by Hou, Chamon, and Mudry [1] that fermion charge fractionalization can take place in monolayer graphene due to Kekulé distortions that are described by means of a complex-valued scalar field (Higgs field) coupled to the Dirac field which, in its turn, describes the dynamics of massless charge carriers in the quantum field theory obtained as the low-energy regime of a discrete model (tight-binding Hamiltonian) of nearest-neighbor hopping on the two-dimensional honeycomb lattice [2,3]. The mechanism for charge fractionalization relies on the existence of zero-energy eigenstates bounded to the vortex associated with the Kekulé distortions that also would open an energy gap at the (two) previously present degeneracy points—two inequivalent Dirac points in the Brillouin zone where the valence and the conduction bands intersect each other—of the tight-binding Hamiltonian. While the so-called valley symmetry is preserved by such midgap bound states, the vorticity of the distortion, either $n \geqslant 1$ or $n \leqslant -1$, determines which one of the two triangular sublattices supports $|n|$ zero modes. That is, the zero modes do not exhibit the so-called pseudospin (sublattice) symmetry presented in both the tight-binding and Dirac Hamiltonians. The zero modes and their sole contribution to the fermion charge fractionalization were shown to persist in a chiral gauge theory for graphene proposed by Jackiw and Pi [4] by adding an axial-vector gauge potential that incorporates axial gauge symmetry [$U_A(1)$] to the field theoretical model in [1].

The chiral coupling of electrons with gauge field in [4] was motivated to give a dynamical origin of the Higgs field, which together with the gauge potential enters in a phenomenological model (Landau-Ginzburg-Abrikosov-Nielsen-Olesen model), whose minimum energy solutions exhibit vortex-like profiles, as those proposed to be realized in graphene. It is worth mentioning that a chiral gauge field was introduced much earlier in the Dirac equation, as an effective equation for charge carriers in a single layer of carbon atoms to describe frustration in fullerenes [5]. Later, Pachos, Stone, and Temme [6] showed that in a honeycomb lattice the modulated hopping strength,

otherwise described by means of a real scalar field, may become a modulated complex-valued field if one considers that the hexagonal lattice has its topology altered, such that the former planar system becomes spherical, as in fullerenes. To take into account the modified topology at the theoretical level, one introduces a chiral gauge field in the Dirac Hamiltonian that describes the low-energy dynamics of charge carriers. In this way, [6] has provided a physical realization of magnetic vortices with fractionalized charge, as those proposed originally in [1] and [4] and also analyzed in detail in [7] and in [8] by taking into account the effects of external magnetic fields.

In a remarkable work [3] dedicated to the role gauge fields might play in the dynamics of charge carriers described by an effective quantum field theory of Dirac fermions, Semenoff showed that the parity anomaly, a phenomenon that was shown to happen in quantum electrodynamics in 2+1 space-time dimensions [9], could be simulated in a planar honeycomb lattice with two species of atoms. In that scenario there is a difference in energies of electrons localized on the different atoms and that implies a parity-violating "mass term" to the field theory effective Hamiltonian that is eventually responsible for the anomalous current that, paraphrasing Semenoff, "would couple to an unphysical external field of abnormal parity and is therefore not directly observable." In other words, that was an axial-vector gauge potential entering in the scene, at least theoretically, in condensed matter, especially in graphite monolayers. Nowadays, it has been proposed that very intense pseudomagnetic fields can be induced by strain in graphene nanobubbles [10] and such pseudomagnetic fields might be associated with the curl of an axial-vector gauge potential nonminimally coupled to Dirac spinors describing the dynamics of electrons in strained graphene.

Indeed, fictitious magnetic fields in graphene have been very fruitful both theoretically and experimentally, as for example in the modeling of corrugations and elastic deformations and in the study of influences that topological defects could lead to in the electronic properties of graphene [11–17]; in the experimental realization of Landau levels in very intense (up to 300 T) pseudomagnetic fields due to stress in strained graphene [10]; and in the possibility to observe, also by means of a scanning-tunneling microscopy, Aharonov-Bohm interferences due to local deformations (microstresses) in graphene [18]. A good review on gauge fields in graphene can

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be found in [19], where the introduction at the theoretical level of elastic deformations, topological defects, and curvature in the low-energy effective Hamiltonian for graphene is reviewed and some of their effects in the electronic properties are discussed (see also [20] and [21]). Fictitious magnetic fields have also been proposed as possible valleys filters in strained graphene [22,23]; a valley filter allows the transmission of a current associated with only one of the valleys, while filters the other one; that is, it transmits a valley-polarized current and constitutes a crucial mechanism in *valleytronics* [24], as much as the spin-filtering mechanism is fundamental to spintronics. In addition, the influence of uniform magnetic and pseudomagnetic fields on the Hall response in graphene samples and the nature of broken-symmetry phases within the lowest Landau levels have been studied in [25].

Motivated by some of the works cited above, we have shown [26] that vector and axial-vector gauge potentials by themselves can bind zero-energy electrons and that fractional charge may be induced even in the absence of Kekulé distortions. In this vein, we have discussed the relation of such induced fractional charge to the parity anomaly which would be realized in gapped graphene as proposed almost thirty years ago [3] and in gapped graphene whose parity symmetry breaking term is provided by the Haldane energy [27]. In addition we also discussed the possible fractionization of another induced quantum number, which we had called chiral charge (number) in the presence of magnetic and pseudomagnetic fields and had briefly shown the connection of the chiral charge to the time component of the abnormal current found in [3].

The chiral charge (number) seems to have an important physical meaning and must be treated as a physical observable in graphene whenever the valley symmetry is preserved at the quantum Hamiltonian level. It is more appropriate to call it the *valley number*, instead. Since the valley symmetry is manifest in this system and there is no intervalley scattering, there is a doubling of fermions for each energy value and it is legitimate to assign to each one-particle state a label (index) to account for the fermion doubling. By its turn, the valley number is defined here as the net number of valley states, i.e., $N_v = N_+ - N_-$, where N_+ is the total number of states (summed over all energy states) around one of the Dirac points, while N_- is the total number of states associated with the other Dirac point.

Here, we consider the sample of graphene in the presence of an external uniform magnetic field and with a local topological defect of disclination type, which is equivalent to a pseudomagnetic field typical of a very thin and long solenoid, the very same magnetic field usually used to discuss the Aharonov-Bohm (AB) effect. In Fig. 1 we show a graphene lattice with the kind of local defect we are interested in (an isolated disclination previously analyzed in [12,28]) and under the action of an external uniform magnetic field. We show that the induced valley number is due only to the zero-energy modes (zero modes) of one-particle states and that there is an imbalance in the number of zero-energy eigenstates associated with the two Dirac points. The presence of the external uniform magnetic field is desirable for many reasons: it can easily realizable in the laboratory, and it provides normalizable zero modes and a Landau level structure for the energy spectrum.
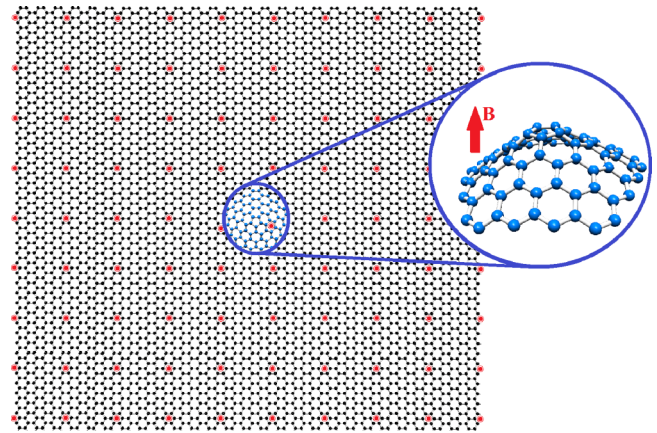

FIG. 1. (Color online) Isolated disclination (blue atoms) in a graphene lattice in the presence of an external uniform magnetic field (red dots) pointing out of the page. The disclination is a consequence of the replacement of the central hexagon by a pentagon. Inset: Detail of the isolated disclination (in perspective), giving rise to a conical geometry with the pentagon close to the apex of the cone; the external magnetic field **B** points upwards.

Notwithstanding, the induced net valley number is shown to be given by $N_v = \pm 1/2(1 - 2\{\Phi/2\pi\})$, where $0 < \{\Phi/2\pi\} < 1$ is the fractional part of the reduced pseudomagnetic flux, whereas the global sign $\pm$ arises from the freedom to choose the zero-energy particles either in the conduction (+) or in the valence (−) band. Some interesting features of this result are the independence of the valley number from the applied external magnetic field, the fractionalization (even irrational values) of the valley number for $\{\Phi/2\pi\} \neq 1/2$, and its null result for $\{\Phi/2\pi\} = 1/2$. Moreover, by extending the concept of valley filtering further, we could say that this is a case of valley-polarized vacuum due to a partial valley filtering, when some of the zero-energy localized states of one of the valleys are filtered. The above result it is not in complete agreement with the one obtained via the field theoretical calculations in the perturbative approach as carried out in [7,26,29]. Within the perturbative approach in field theory one would obtain $N_v = \pm \Phi/2\pi$ whether the pseudomagnetic flux is integer or not, but it depends on the Pauli-Villars regulator used to regularize the induced Chern-Simons action. Then the nonperturbative field theoretical calculation carried out here, namely, by using the canonical operator formalism and the exact one-particle states, is important, because it reveals some features which probably cannot be attained via the usual perturbative approach.

In the next section we discuss the one-particle states by solving the proper Dirac equation we have in hand and comment on the relevant symmetries of the problem. In the third section we present the second quantization of the fermion field, comment on the manifest valley symmetry in the context of quantum field theory, calculate the induced valley number, and show that one may have quasiparticles carrying fractional *valley charge*. We also compute the induced electric charge in this context.

To show the similarity of that supposed partial valley filtering to a partial spin filtering also in graphene, in the fourth section we consider the very same configurations of magnetic

and pseudomagnetic fields in the effective Hamiltonian for low-energy electrons whenever the valley degree of freedom is decoupled and the relevant degrees of freedom are the pseudospin (associated to the two triangular sublattices) and the spin polarization. There we do not take into account the antiferromagnetic order as it was considered in [30], because that would break the spin symmetry at the Hamiltonian level, which would not give reliability to the spin polarization of the field as a physical observable. We show that the filtering of some zero-energy states of spin polarization implies quasiparticles carrying fractional, even irrational, spin polarization. The fifth section is left to further comments on the results we have found and a short analysis about the possible induction of fractional valley number in strained and in *in-plane* deformed graphene samples.

II. BOUND STATES ON MAGNETIC AND PSEUDOMAGNETIC FIELDS

The effective field theory Hamiltonian describing the dynamics of the electrons on the graphene honeycomb structure in the presence of an external magnetic field $\vec{B}_V = \vec{\nabla} \times \vec{V}$ and a pseudomagnetic field $\vec{B}_A = \vec{\nabla} \times \vec{A}$ can be written as

$$\mathcal{H} = \int d^2\vec{r}\, \Psi^\dagger(\vec{r},t) \hat{h}_D \Psi(\vec{r},t), \qquad (1)$$

where $\hat{h}_D = \vec{\alpha} \cdot (-i\vec{\nabla} - e\vec{V} - \gamma_5 \vec{A})$ is the Dirac Hamiltonian operator and $\Psi(\vec{r})$ is a four-component spinor, whose transpose is $\Psi^T = (\psi_+^b \, \psi_+^a \, \psi_-^a \, \psi_-^b)$. The superscripts a and b in the spinor components designate the triangular sublattices on which the electrons are supported, while the subscripts $\pm$ stand for each one of the two inequivalent Dirac points. The matrix structure in (1) is made explicit by means of the following matrices:

$$\beta = \begin{pmatrix} 0 & I \\ I & 0 \end{pmatrix}, \quad \vec{\alpha} = \begin{pmatrix} \vec{\sigma} & 0 \\ 0 & -\vec{\sigma} \end{pmatrix},$$

$$\alpha^3 = \begin{pmatrix} \sigma_3 & 0 \\ 0 & -\sigma_3 \end{pmatrix}, \quad \gamma_5 = -i\alpha^1\alpha^2\alpha^3 = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}, \qquad (2)$$

where I is the 2×2 identity matrix and $\vec{\sigma} = (\sigma_1, \sigma_2)$ and σ_3 are the Pauli matrices in the standard representation.

We notice that (1) is invariant under local $U(1) \times U_A(1)$ gauge transformations $\Psi \to e^{i[e\vartheta(\vec{x}) + \gamma_5\omega(\vec{x})]}\Psi$, $\vec{V} \to \vec{V} + \vec{\nabla}\vartheta(\vec{x})$, and $\vec{A} \to \vec{A} + \vec{\nabla}\omega(\vec{x})$. Moreover, because we are in $(2+1)$ dimensions, the chiral anomaly is absent.

The corresponding time-independent Dirac equation

$$\hat{h}_D \Psi(\vec{r},t) = E\Psi(\vec{r},t) \qquad (3)$$

can be decomposed in two independent Dirac equations, for the upper $\psi_+^T = (\psi_+^b \psi_+^a)$ and lower $\psi_-^T = (\psi_-^a \psi_-^b)$ components of the energy eigenfunctions, that are associated with each one of the Dirac points in the Brillouin zone of the honeycomb lattice:

$$[(\pm\vec{\sigma}) \cdot \vec{\Pi}_\pm]\psi_\pm(\vec{r},t) = E\psi_\pm(\vec{r},t), \qquad (4)$$

with $\vec{\Pi}_\pm = -(i\vec{\nabla} + e\vec{V} \pm \vec{A})$.

The bispinors $\Psi_+^T = (\psi_+^T 0)$ and $\Psi_-^T = (0\psi_-^T)$ are also eigenstates of γ_5 that commute with the Dirac Hamiltonian operator, with eigenvalues ± 1, respectively. This is the manifestation of the valley symmetry at the quantum mechanics

level. Furthermore, once the Dirac Hamiltonian operator anticommutes with α^3 and with $\alpha^3\gamma_5$, the energy spectrum is symmetric around the zero-energy level. In other words, if there is a norm-preserving operator (unitary operator $\mathcal{C}$) such that $\{\hat{h}_D, \mathcal{C}\} = 0$, then for each positive-energy normalized eigenstate, $\Psi_{|E|}$, there is one corresponding negative-energy normalized eigenstate $\Psi_{-|E|} = \mathcal{C}\Psi_{|E|}$ and the zero modes are self-conjugate.

When the external magnetic field is uniform and one considers that the graphene sheet is under disclination, the vector and axial-vector potentials can be written in the symmetric gauges respectively as

$$V^i = -\frac{B}{2}\varepsilon^{ij}x^j, \quad A^i = -\frac{\Phi}{2\pi r^2}\varepsilon^{ij}x^j, \qquad (5)$$

where $\varepsilon^{12} = -\varepsilon^{21} = 1$ and $\Phi = \int d^2\vec{r}\, B_A$ is the flux of the pseudomagnetic field $B_A = \Phi\delta(r)/2\pi r$ (in cylindrical coordinates), which exhibits the same profile of the magnetic field used to describe the AB effect. Such effect involves a charged particle in the presence of a background magnetic field concentrated within a flux tube where the probability of the particle be found is zero. Here, it is the topological defect that is represented by such (pseudo)magnetic field (see [12,28]).

The zero-energy normalized eigenfunctions associated with the electrons under the above magnetic and pseudomagnetic fields are given by

$$\Psi_{0,l,+}(\vec{r}) = \sqrt{\frac{|eB/2|^{1+l-\frac{\Phi}{2\pi}}}{\pi\Gamma\left(1+l-\frac{\Phi}{2\pi}\right)}} \begin{pmatrix} e^{il\theta} \\ 0 \\ 0 \\ 0 \end{pmatrix} r^{l-\frac{\Phi}{2\pi}} e^{-\frac{|eB|}{4}r^2},$$

$$\Psi_{0,k,-}(\vec{r}) = \sqrt{\frac{|eB/2|^{1+k+\frac{\Phi}{2\pi}}}{\pi\Gamma\left(1+k+\frac{\Phi}{2\pi}\right)}} \begin{pmatrix} 0 \\ 0 \\ e^{ik\theta} \\ 0 \end{pmatrix} r^{k+\frac{\Phi}{2\pi}} e^{-\frac{|eB|}{4}r^2}, \qquad (6)$$

for $eB > 0$, and by

$$\Psi_{0,l,+}(\vec{r}) = \sqrt{\frac{|eB/2|^{1+l+\frac{\Phi}{2\pi}}}{\pi\Gamma\left(1+l+\frac{\Phi}{2\pi}\right)}} \begin{pmatrix} 0 \\ e^{-il\theta} \\ 0 \\ 0 \end{pmatrix} r^{l+\frac{\Phi}{2\pi}} e^{-\frac{|eB|}{4}r^2},$$

$$\Psi_{0,k,-}(\vec{r}) = \sqrt{\frac{|eB/2|^{1+k-\frac{\Phi}{2\pi}}}{\pi\Gamma\left(1+k-\frac{\Phi}{2\pi}\right)}} \begin{pmatrix} 0 \\ 0 \\ 0 \\ e^{-ik\theta} \end{pmatrix} r^{k-\frac{\Phi}{2\pi}} e^{-\frac{|eB|}{4}r^2}, \qquad (7)$$

for $eB < 0$. In the above expressions, θ is the angular variable in cylindrical coordinates and $l, k \in \mathbb{Z}$, with $l > \Phi/2\pi - 1$ and $k > -\Phi/2\pi - 1$ (for $eB > 0$), which are conditions to get normalized states. For $eB < 0$ one must have $l > -\Phi/2\pi - 1$ and $k > \Phi/2\pi - 1$. From these conditions one can note that there are infinite zero modes in both valleys, and that the pseudomagnetic field causes the lower bound of k to be less than that of l in the case $\Phi > 0$ and $eB > 0$. This leads us to conjecture that there are additional states of $\Psi_{0,k,-}$ with respect to $\Psi_{0,l,+}$, and vice versa in the case $\Phi < 0$. One can check that the external uniform magnetic field not only provides normalizable zero modes, but also brings the imbalance on the number of

zero modes out. In fact, in the absence of it both valleys support $[\Phi/2\pi] - 1$ singular zero modes [26,31,32] ($[\Phi/2\pi] > 0$ is the integer part of the reduced pseudomagnetic flux).

Solutions of the Dirac equations as those in (4) for the scattering of massive fermions (when a mass term $m\sigma^3$ is added to the Dirac Hamiltonian operator) by only an AB-like magnetic field were discussed in several papers, for instance [33–35], and of massless fermions in [36]. In our case, the presence of the uniform magnetic field changes the energy spectrum of the particle from a continuous spectrum to a discrete one. Our treatment to reach the excited states, $E \neq 0$, follows the one given in [37,38], where we find a discussion of the wave functions of massive fermions in the presence of a uniaxial magnetic field with two contributions, a uniform magnetic field and the AB-like magnetic field. Parenthetically we notice that each one of the equations in (4) corresponds exactly to the equations solved in [37,38], except that we are interested in massless fermions and that the ground states were obtained here through the first-order differential equations (4), while the second-order differential equations are used in [37,38] to obtain all the eigenstates, but the irregular ones at the origin. (For the sake of simplicity we use a specific value of the adjoint extension parameter; any other choice does not modify the main results presented in the next section.)

The orthonormal eigenstates of positive energy, angular momentum, and of γ_5 can be worked out straightforwardly and have the forms

$$\Psi_{|E_+|,l,+}(\vec{r}) = \frac{e^{il\theta}}{\sqrt{2}} \begin{pmatrix} R_{n,\nu_+}(r) \\ i R_{n-1,\nu_++1}(r) \\ 0 \\ 0 \end{pmatrix},$$

$$\Psi_{|E_-|,k,+}(\vec{r}) = \frac{e^{ik\theta}}{\sqrt{2}} \begin{pmatrix} 0 \\ 0 \\ R_{n,\nu_-}(r) \\ -i R_{n-1,\nu_-+1}(r) \end{pmatrix}, \tag{8}$$

where $\nu_+ = l - \Phi/2\pi$, $\nu_- = k + \Phi/2\pi$, and

$$R_{n,\nu}(r) = \sqrt{\frac{(|eB|/2)^{1+\nu} n!}{\pi \Gamma(n+\nu+1)}} r^\nu e^{-\frac{|eB|}{4}r^2} L_n^\nu(\gamma r^2) \tag{9}$$

are the Gauss Laguerre modes in cylindrical coordinates conveniently constructed such that $\int |R_{n,\nu}(r)|^2 d^2\vec{r} = 1$, and we are assuming that $R_{-1,\nu}(r) = 0$ and $\nu > 1$.

The bound state solutions for $\nu_\pm < -1$ are given by

$$\Psi_{|E_+|,l,+}(\vec{r}) = \frac{e^{il\theta}}{\sqrt{2}} \begin{pmatrix} R_{n,|\nu_+|}(r) \\ -i R_{n,|\nu_+|-1}(r) \\ 0 \\ 0 \end{pmatrix},$$

$$\Psi_{|E_-|,k,-}(\vec{r}) = \frac{e^{ik\theta}}{\sqrt{2}} \begin{pmatrix} 0 \\ 0 \\ R_{n,|\nu_-|}(r) \\ i R_{n,|\nu_-|-1}(r) \end{pmatrix}, \tag{10}$$

while the eigenstates of negative energy with $\nu_\pm > +1$ and $\nu_\pm < -1$ can be obtained by applying the unitary operator α^3 to the eigenstates (8) and (10), respectively.

The subscripts $|E_\pm|$ designate the energy eigenvalues which are the Landau levels (LLs)

$$|E_\pm| = \sqrt{2eBn},$$

$$\text{with } n = 1,2,3,\ldots \text{ for } \begin{cases} l \geq 2 + [\Phi/2\pi] \\ k \geq 1 - [\Phi/2\pi] \end{cases} \tag{11}$$

that are obtained from the regularity condition $\nu_\pm > +1$, while from $\nu_\pm < -1$ one obtains

$$|E_\pm| = \sqrt{2eB(n - m \pm \Phi/2\pi)} \ \ (n = 0,1,2,\ldots), \tag{12}$$

where m stands for $l \leq -1 + [\Phi/2\pi]$ in case of $|E_+|$ and for $k \leq -2 - [\Phi/2\pi]$ in case of $|E_-|$.

Only regular eigenfunctions have been considered so far. The irregular ones, corresponding to $\nu_+ = -\{\Phi/2\pi\}, 1 - \{\Phi/2\pi\}$ and to $\nu_- = \{\Phi/2\pi\}, -1 + \{\Phi/2\pi\}$ ($0 < \{\Phi/2\pi\} < 1$ is the fractional part of the reduced pseudomagnetic flux) are obtained from the first-order differential equations (4). We have found that the irregular eigenstates $\Psi_{|E_+|,1+[\frac{\Phi}{2\pi}],+}$ and $\Psi_{|E_-|,-[\frac{\Phi}{2\pi}],-}$ have their corresponding energy eigenvalues in the set (11), whereas for $\Psi_{|E_+|,[\frac{\Phi}{2\pi}],+}$ and $\Psi_{|E_-|,-1-[\frac{\Phi}{2\pi}],-}$ the corresponding energy eigenvalues belong to the set (12).

Notice that the LLs (including the zero-energy level) are degenerate with respect to eigenstates of γ_5 and $\hat{L} = -i\partial_\theta$. For the zero-energy level, one has $l \geqslant [\Phi/2\pi]$ and $k \geqslant -1 - [\Phi/2\pi]$, and the LL one has $l \geq 1 + [\Phi/2\pi]$ and $k \geq -[\Phi/2\pi]$, due to the irregular eigenstates. The energy levels in the set (12) with $l \leq [\Phi/2\pi]$ and $k \leq -1 - [\Phi/2\pi]$ may be degenerate only for $\{\Phi/2\pi\} = 1/2$. Moreover, one only has a complete set of eigenstates if the zero-energy eigenstates with $l = [\Phi/2\pi]$ and $k = -1 - [\Phi/2\pi]$ are dropped out from the set of eigenstates. This complete set of eigenstates comprises the basis from which the fermion field operator will be built in the next section.

III. INDUCED VALLEY NUMBER

In this section we focus on the computation of the induced valley number that is defined here as the vacuum expectation value of the valley number operator, namely

$$\hat{N}_\text{v} = \frac{1}{2} \int d^2\vec{r} [\hat{\Psi}^\dagger(\vec{r},t), \gamma_5 \hat{\Psi}(\vec{r},t)], \tag{13}$$

where $\hat{\Psi}^\dagger(\vec{r},t)$ is the fermion field operator that is expanded on the basis of the one-particle states presented in the previous section in the following way:

$$\begin{aligned}
\widehat{\Psi}(\vec{r},t) = &\sum_{l=[\Phi/2\pi]+1}^{+\infty} \tilde{\mathbf{c}}_{0,l,+} \Psi_{0,l,+}(\vec{r}) + \sum_{k=-[\Phi/2\pi]}^{+\infty} \tilde{\mathbf{c}}_{0,k,-} \Psi_{0,k,-}(\vec{r}) \\
&+ \sum_{n=0}^{+\infty} \Bigg\{ \sum_l [\mathbf{c}_{n,l,+} \Psi_{|E_+|,l,+}(\vec{r}) e^{-i|E_+|t} \\
&+ \mathbf{d}_{n,l,+}^\dagger \alpha^3 \Psi_{|E_+|,l,+}(\vec{r}) e^{+i|E_+|t}] \\
&+ \sum_k [\mathbf{c}_{n,k,-} \Psi_{|E_-|,k,-}(\vec{r}) e^{-i|E_-|t} \\
&+ \mathbf{d}_{n,k,-}^\dagger \alpha^3 \Psi_{|E_-|,k,-}(\vec{r}) e^{+i|E_-|t}] \Bigg\}.
\end{aligned} \tag{14}$$

In this expansion of the fermion field $\mathbf{c}_{n,m,\mathrm{v}}$ ($\mathbf{d}_{n,m,\mathrm{v}}^{\dagger}$) is the absorption (creation) operator of a particle of energy $|E_{\pm}|$, angular momentum $m = l,k$ and valley $\mathrm{v} = \pm$ in the conduction (valence) band. The energies $|E_{\pm}|$ of the particles are given by expressions (11) and (12) with the corresponding values l and k assumed. The particles of zero energy are, by construction of the fermion field, supposed to be in the conduction band and their absorption operators are represented by $\tilde{\mathbf{c}}_{0,m,\mathrm{v}}$. The creation $\mathbf{d}_{n,m,\mathrm{v}}^{\dagger}$ ($\mathbf{c}_{n,m,\mathrm{v}}^{\dagger}$) and absorption $\mathbf{d}_{n,m,\mathrm{v}}$ ($\mathbf{c}_{n,m,\mathrm{v}}$) operators of particles in the valence (conduction) band obey the following anticommutation relations:

$$\{\mathbf{c}_{n,m,\mathrm{v}},\mathbf{c}_{n',m',\mathrm{v}'}^{\dagger}\} = \{\mathbf{d}_{n,i},\mathbf{d}_{n',i'}^{\dagger}\} = \delta_{nn'}\delta_{mm'}\delta_{\mathrm{vv}'},$$
$$\{\tilde{\mathbf{c}}_{0,m,\mathrm{v}},\tilde{\mathbf{c}}_{0,m',\mathrm{v}'}^{\dagger}\} = \delta_{mm'}\delta_{\mathrm{vv}'}, \tag{15}$$

with all the others possible anticommutators vanishing. Then, one can show that $\{\widehat{\Psi}^{\dagger}(\vec{r},t),\widehat{\Psi}(\vec{r}',t)\} = \delta^{2}(\vec{r} - \vec{r}')$, since one has a complete set of eigenfunctions as that developed in the previous section.

Then, the valley number operator can be expressed as $\hat{N}_{\mathrm{v}} = \hat{N}_{+} - \hat{N}_{-}$, where

$$\hat{N}_{+} = \sum_{l=[\Phi/2\pi]+1}^{+\infty}\left(\tilde{\mathbf{c}}_{0,l,+}^{\dagger}\tilde{\mathbf{c}}_{0,l,+} - \frac{1}{2}\int d^{2}\vec{r}|\Psi_{0,l,+}|^{2}\right)$$
$$+ \sum_{n}\sum_{l=-\infty}^{+\infty}(\mathbf{c}_{n,l,+}^{\dagger}\mathbf{c}_{n,l,+} - \mathbf{d}_{n,l,+}^{\dagger}\mathbf{d}_{n,l,+}), \tag{16}$$

$$\hat{N}_{-} = \sum_{k=-[\Phi/2\pi]}^{+\infty}\left(\tilde{\mathbf{c}}_{0,k,-}^{\dagger}\tilde{\mathbf{c}}_{0,k,-} - \frac{1}{2}\int d^{2}\vec{r}|\Psi_{0,k,-}|^{2}\right)$$
$$+ \sum_{n}\sum_{k=-\infty}^{+\infty}(\mathbf{c}_{n,k,-}^{\dagger}\mathbf{c}_{n,k,-} - \mathbf{d}_{n,k,-}^{\dagger}\mathbf{d}_{n,k,-}) \tag{17}$$

are the fermion number operators associated with the valley $+$ and valley $-$, respectively. In obtaining these expressions one must remember that for each positive-energy state of a given valley there is a corresponding negative-energy state, such that they cancel each other. Furthermore, one can note that each of the fermion number operators acquires a c-number contribution whose origin is due to the zero

modes; i.e.,

$$c\text{ number}_{+} = \int d^{2}\vec{r}\rho_{+}(\vec{r}) = -\frac{1}{2}\int d^{2}\vec{r}\sum_{l=[\Phi/2\pi]+1}^{+\infty}|\Psi_{0,l,+}|^{2}$$
$$= -\frac{1}{2}\int_{0}^{+\infty}d\zeta e^{-\zeta}\sum_{l=[\Phi/2\pi]+1}^{+\infty}\frac{\zeta^{l-\Phi/2\pi}}{\Gamma(1+l-q\Phi/2\pi)}$$
$$= -\frac{1}{2}\int_{0}^{+\infty}d\zeta\left(1 + \frac{\zeta^{-\{\Phi/2\pi\}}e^{-\zeta}}{\Gamma(1-\{\Phi/2\pi\})}\right.$$
$$\left. - \frac{\Gamma(1-\{\Phi/2\pi\},\zeta)}{\Gamma(1-\{\Phi/2\pi\})}\right)$$
$$= -\frac{1}{2}\left(\{\Phi/2\pi\} + \int_{0}^{+\infty}d\zeta\right), \tag{18}$$

$$c\text{ number}_{-} = \int d^{2}\vec{r}\rho_{-}(\vec{r}) = -\frac{1}{2}\int d^{2}\vec{r}\sum_{k=-[\Phi/2\pi]}^{+\infty}|\Psi_{0,k,-}|^{2}$$
$$= -\frac{1}{2}\int_{0}^{+\infty}d\zeta e^{-\zeta}\sum_{k=-[\Phi/2\pi]}^{+\infty}\frac{\zeta^{k+\Phi/2\pi}}{\Gamma(1+k+\Phi/2\pi)}$$
$$= -\frac{1}{2}\int_{0}^{+\infty}d\zeta\left(1 + \frac{\zeta^{\{\Phi/2\pi\}-1}e^{-\zeta}}{\Gamma(\{\Phi/2\pi\})}\right.$$
$$\left. - \frac{\Gamma(\{\Phi/2\pi\},\zeta)}{\Gamma(\{\Phi/2\pi\})}\right)$$
$$= -\frac{1}{2}\left((1 - \{\Phi/2\pi\}) + \int_{0}^{+\infty}d\zeta\right), \tag{19}$$

where $\Gamma(\alpha,\zeta)$ is the upper incomplete Gamma function [39], with $\zeta = eBr^{2}/2$. The c numbers are the only ones responsible for the nonvanishing vacuum expectation of the fermion numbers associated with each one of valleys. Figure 2 shows the absolute values of $\rho_{+}(\vec{r})$, $\rho_{-}(\vec{r})$ and of the difference $\rho(\vec{r}) = \rho_{+}(\vec{r}) - \rho_{-}(\vec{r})$ in dimensionless units, where one can appreciate the sharp behavior of the the "valley number densities" around the defect.

As a consequence of those contributions, each one of the fermion numbers picks up a nonvanishing vacuum expectation, namely $N_{+} = \langle 0|\hat{N}_{+}|0\rangle = -(\frac{\Phi_{B}}{4\pi} + \{\frac{\Phi}{4\pi}\})$ and $N_{-} = \langle 0|\hat{N}_{-}|0\rangle = -(\frac{\Phi_{B}}{4\pi} + \frac{1}{2} - \{\frac{\Phi}{4\pi}\})$, where $\Phi_{B}/2\pi$ is the reduced flux of the external magnetic field which is not quantized; it is infinity in fact once B_{V} is uniform and in the calculations we
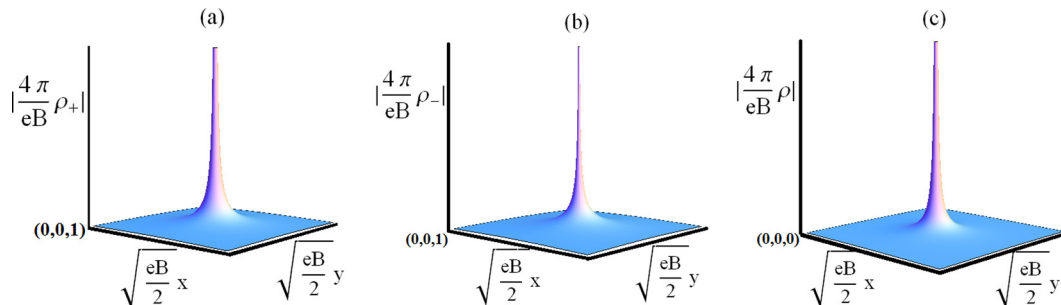

FIG. 2. (Color online) Absolute values of (a) surface density ρ_{+}, Eq. (18); (b) surface density ρ_{-}, Eq. (19); (c) net surface density (net valley number density) $\rho = \rho_{+} - \rho_{-}$ as functions of the coordinate r (in dimensionless units).

have done so far the graphene sample has infinity dimensions [$r \in [0,\infty)$]. As one can see, there is an induced fermion charge associated with each one of the valleys due to the magnetic fields, whose results are compatible with the results of the induced electric charge and parity anomaly in QED in 2+1 dimensions. In fact, the total induced charge of the system—which is also a physical observable and may be fractional when specific configurations of the magnetic and pseudomagnetic fields are considered and is fractional under Kekulé deformations—is

$$Q = \langle 0|\hat{Q}|0\rangle = -\frac{e}{2}\left(-1 + 2e\frac{\Phi_B}{2\pi}\right). \qquad (20)$$

From the above expression one sees that this induced charge is infinity once the flux of the external and uniform magnetic field is infinity, but it also has a fractional contribution $e/2$ due to the AB-like pseudomagnetic field.

On the other hand the induced valley number is finite and given by

$$N_{\rm v} = \langle 0|\hat{N}_{\rm v}|0\rangle = \langle 0|\hat{N}_+ - \hat{N}_-|0\rangle = \frac{1}{2} - \left\{\frac{\Phi}{2\pi}\right\}. \qquad (21)$$

That is a measure of the imbalance on the number of zero modes among the valleys. Parenthetically we notice that we would obtain $N_{\rm v} = -1/2(1 - 2\{\Phi/2\pi\})$ had we considered the zero-energy particles in the valence band. Although $N_{\rm v}$ does not depend explicitly on the applied uniform magnetic field, one would obtain $N_{\rm v} = 0$ in the absence of the external field, for the number of zero modes on both valleys is the same and, for the same reason, Q would be finite and equals $e/2$.

Another consequence of the c number as it stands in (18) and in (19) is that each particle in the conduction or in the valence band would carry a fractional valley charge as follows:

$$\begin{aligned}
&\hat{N}_{\rm v}\,|1_{\rm cond},n,m,\pm\rangle \\
&= \hat{N}_{\rm v}\mathbf{c}^\dagger_{n,m,\pm}\,|0\rangle \\
&= [\pm 1 + 1/2(1 - 2\{\Phi/2\pi\})]\,|1_{\rm cond},n,m,\pm\rangle, \\
&\hat{N}_{\rm v}\,|1_{\rm val},n,m,\pm\rangle \\
&= \hat{N}_{\rm v}\mathbf{d}^\dagger_{n,m,\pm}\,|0\rangle \\
&= [\mp 1 + 1/2(1 - 2\{\Phi/2\pi\})]\,|1_{\rm val},n,m,\pm\rangle.
\end{aligned}$$

From this last result one can see that, except for the zero-energy states, to each particle in the valence band and in the valley $+$ $(-)$ is assigned the same valley charge of a particle in the conduction band and in the valley $-$ $(+)$.

Had we started with the Haldane mass term in $\hat{h}_D$ ($m_H\alpha^3\gamma_5$), we would have obtained $N_{\rm v} = \frac{m_H}{|m_H|}(\frac{1}{2} - \{\frac{\Phi}{2\pi}\})$ and the sign ambiguity is accounted for the sign of mass. In the perturbative approach, by calculating the vacuum polarization Feynman diagrams and by using the Haldane mass term as the Pauli-Villars regulator the result would be a little bit different ($N_{\rm v} = \lim_{m_H \to 0}\frac{m_H}{|m_H|}\frac{\Phi}{2\pi}$), because in the perturbative approach an equal number of zero modes on both of the valleys is assumed *a priori*.

IV. FRACTIONAL (EVEN IRRATIONAL) SPIN POLARIZATION

In this section we discuss the analogy between induced valley number and induced spin polarization in graphene in order to reinforce the development of valleytronics in analogy to spintronics. In valleytronics the pseudomagnetic fields due to topological defects, microstresses, and deformations in clean graphene samples had shown to be useful in the filtering mechanism which selects valley-polarized electric currents as much as spin-polarized currents are produced in the context of spintronics.

In the previous two sections we have not considered the spin degrees of freedom, since in clean samples of graphene there is no room for spin-spin interaction or spin flipping in graphene. In the present section we decouple the two valley degrees of freedom from the full Dirac Hamiltonian that describes the low-energy dynamics of electrons in the honeycomb lattice and we are left with the pseudospin (sublattices a and b) and spin degrees of freedom. By following [30] we write the following quantum mechanics Dirac Hamiltonian operator:

$$\hat{h} = i(\vec{\sigma}\otimes I)\cdot[\vec{\nabla} - ie\vec{V} - i(I\otimes\tau_3)\vec{A}]. \qquad (22)$$

The 4×4 matrix structure of $\hat{h}$ comes from the direct product of 2×2 matrices; one of the sets, namely the identity matrix I and the Pauli matrices σ^i, is associated with the pseudospin, while the other one is formed by the identity matrix and the spin Pauli matrices τ^a. Moreover, $\vec{V}$ is the vector gauge potential associated with the external magnetic field and $\vec{A}$ is the axial-vector gauge potential associated with the pseudomagnetic field. In order to carry the analogy of induced valley number and induced spin polarization further and show that the spin polarization can be fractional as a consequence of the imbalance on the number of zero modes with different spin polarizations, we consider that the gauge potentials have the same configurations as given in (5).

Because $\hat{h}$ commutes with the spin polarization operator $I\otimes\tau_3$, one can label the energy eigenstates as $\Psi_\pm = \frac{1}{2}(1\pm\sigma_3)\otimes I\Psi$, where Ψ_+ and Ψ_- are eigenstates of $I\otimes\tau_3$ also, with eigenvalues $+1$ and -1, respectively. Moreover, $\hat{h}$ anticommutes with $\mathcal{C} = \sigma_3\otimes\tau_3$; then if $\Psi_\pm^E$ is an eigenstate of $\hat{h}$ with eigenvalue $E \neq 0$, $\mathcal{C}\Psi_\pm^E$ is also an eigenstate of $\hat{h}$ with eigenvalue $-E$, and the zero modes are $\mathcal{C}$ self-conjugate. With such considerations one can find the explicit form of the eigenstates of $\hat{h}$, $I\otimes\tau_3$, and $\hat{L} = -i\partial_\theta$ as they were found in Sec. II. Moreover, according to the steps developed in the previous section, only the zero modes matter to the calculation of the vacuum expectation value. Then, for the sake of simplicity we present only them here, namely

$$\Psi_{0,+,l} = \sqrt{\frac{(eB/2)^{1+l-\frac{\Phi}{2\pi}}}{\pi\,\Gamma\left(1 + l - \frac{\Phi}{2\pi}\right)}}\begin{pmatrix}e^{il\theta}\\0\\0\\0\end{pmatrix}r^{l-\frac{\Phi}{2\pi}}e^{-eBr^2/2},$$

$$\Psi_{0,k,-}(\vec{r}) = \sqrt{\frac{(eB/2)^{1+k+\frac{\Phi}{2\pi}}}{\pi\,\Gamma\left(1 + k + \frac{\Phi}{2\pi}\right)}}\begin{pmatrix}0\\e^{ik\theta}\\0\\0\end{pmatrix}r^{k+\frac{\Phi}{2\pi}}e^{-\frac{eB}{4}r^2}.$$

$$(23)$$

We notice that the only thing that distinguishes these zero-energy eigenstates from those in (6) is their matrix structure. The same happens to the other eigenstates. In other words, eigenstates $\Psi_{|E|,+,l}$ ($\Psi_{|E|,-,k}$) have in general the first and the third (the second and the fourth) components different from zero. The energy eigenvalues are given by (11) and (12).

Since the quantum field operator

$$\hat{S} = \frac{1}{2} \int d^2\vec{r}\,[\hat{\Psi}^\dagger(\vec{r},t), I \otimes \tau_3 \hat{\Psi}^\dagger(\vec{r},t)] \qquad (24)$$

commutes with the quantum field theory Hamiltonian operator

$$\hat{H} = \frac{1}{2} \int d^2\vec{r}\,\{\hat{\Psi}^\dagger(\vec{r},t), i(\vec{\sigma} \otimes I)$$
$$\cdot[\vec{\nabla} - ie\vec{V} - i(I \otimes \tau_3)\vec{A}]\hat{\Psi}^\dagger(\vec{r},t)\}, \qquad (25)$$

it can be associated with a physical observable. Then, by following the same steps of Sec. III one finds the induced spin polarization as given by

$$S = \langle 0|\hat{S}|0\rangle = \frac{1}{2} - \left\{\frac{\Phi}{2\pi}\right\}. \qquad (26)$$

One can check that the (quasi)particles would carry fractional (even irrational) spin polarization. This result must be understood only as an illustrative analogy to the result on the fractional valley number due to topological defects in the graphene lattice, because topological defects do not affect the spin polarization degree of freedom.

V. FURTHER COMMENTS AND CONCLUSIONS

We have analyzed the influence of an external magnetic field in a clean graphene sheet with a local topological defect (single disclination). Such a topological defect can be described in the low-energy continuum model for the charge carriers as a Aharonov-Bohm-like pseudomagnetic field whose axial-vector gauge potential couples to the two valley degrees of freedom with different signs. As a consequence of this and due to the configuration of the pseudomagnetic field one has a partial breaking of the valley symmetry originally present in the low-energy effective Hamiltonian for the charge carriers. This partial breaking of the valley symmetry is revealed in the energy spectrum of the system which is no longer the usual (degenerate) Landau levels (LLs) for a (relativistic) massless fermion in a uniform magnetic field. For instance, between the zero-energy level and the first LL with energy $\sqrt{2eB}$, there appears two additional nondegenerate energy levels with energies $\sqrt{2eB\{\Phi/2\pi\}}$ and $\sqrt{2eB(1 - \{\Phi/2\pi\})}$ ($0 < \{\Phi/2\pi\} < 1$ is the fractional part of the reduced pseudomagnetic flux); each one of these intermediary energy levels contains a unique member of only one of the valleys. In addition, each one of the LLs is partially degenerate as regards the valley degree of freedom; namely, there is an imbalance in the number of valley states on those energy levels. A measure of this imbalance, which we have called a partial filtering, can be defined in the context of quantum field theory as the valley number given by the vacuum expectation value of the number operator associated with one of the valleys minus the expectation value of the number operator associated with the other valley. We have analyzed that in the third section

and have shown that due to the sole contribution of the zero modes, the valley number is in fact finite and may be fractional (even irrational) for $\{\Phi/2\pi\} \neq 1/2$. To show that the sum of states is infinity, specifically concerning the zero-energy states, we have also computed the induced electric charge and have shown that it is proportional do the flux of the external magnetic field, which is infinity because the external field is uniform and the graphene sample is taken to be infinity. This last result would be expected from the parity anomaly in QED in 2+1 space-time dimensions. In fact, in the absence of intervalley scattering, the continuum model for the dynamics of charge carriers in graphene in magnetic and pseudomagnetic fields may be seen as two decoupled QED in 2+1 dimensions (one for each valley degree of freedom) for massless fermions.

The above splitting on the lowest LL may be a good candidate to explain the degeneracy lift of the zero-energy level and perhaps the appearance of a mass gap, that has been observed in graphene samples under relatively strong magnetic fields. Since it seems to be very difficult to have a perfect, free-of-defects graphene sample, the influence of those kind of topological defects enhanced by a relatively strong magnetic field might be observed.

We have also wondered whether similar effects could also take place in strained samples of graphene under microstresses, as those reported in [10] where uniform (pseudo)magnetic fields up to 300 T seems to be realized. In view of the results in [25,26], we conclude that particles associated with the different valleys would describe orbits with different cyclotron frequencies, namely $\omega_\pm = |eB \pm B_A|/2$ and each Landau level, say $\sqrt{2eBn}$, is split in two levels with energies $\sqrt{|eB + B_A|n}$ and $\sqrt{|eB - B_A|n}$; each one contains a representative of only one of the valleys. The zero-energy level still persists with representatives of both valleys, but since they have different cyclotron frequencies, there will be an induced valley number given by $N_v = \pm\Phi/2\pi$ (the ambiguity of the sign is attributed to the zero-energy particles assigned to the valence or to the conduction band), which is no longer fractional; neither is it finite once the pseudomagnetic field is uniform and the sample is taken to be infinitely large. An interesting aspect of these results is that now we are able, by fine-tuning the external magnetic field, to filter one of the valleys completely and leading to *valley-polarized* cyclotron orbits and to *chiral eddy currents*.

We have also analyzed other kinds of deformations in graphene, such as the symmetric in-plane ones [18], but we have not been able to reach a definite conclusion in favor of partial filtering in this case. Nevertheless, in view of the results presented here and based on the index theorems on the number of zero modes of the Dirac Hamiltonian [40–42], we believe that a partial valley filtering and a non-null induced valley number take place whenever there is a net pseudomagnetic flux. Then, as an example of the kinds of in-plane deformation analyzed in [18], we have considered a pseudomagnetic field given by $B_A = \frac{-\kappa u_{00}\Phi_0}{\pi\sigma^6}(r^4 - 7\sigma^2 r^2 + 4\sigma^4)e^{-r^2/2\sigma^2}$ whose flux is $\Phi = 4\kappa u_{00}\Phi_0$; we would expect that, even in the background of the uniform magnetic field, for which the index theorem seems not to be applicable, since one has an infinite flux [42],

an induced valley number given by $N_{\rm v} = \pm 2\kappa u_{00}\Phi_0$, where Φ_0 is the quantum of flux and $\kappa u_{00} = 0.3$ from the data in [18]. An identical result is expected from field theoretical calculations within the perturbative approach, as those carried out in [7,26,29], if one uses the Haldane mass term as the Pauli-Villars regulator, because in this case there is no imbalance on the number of one-particle zero-energy states.

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