Chiral anomaly and anomalous finite-size conductivity in graphene

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Abstract

Graphene is a monolayer of carbon atoms packed into a hexagon lattice to host two spin degenerate pairs of massless two-dimensional Dirac fermions with different chirality. It is known that the existence of non-zero electric polarization in reduced momentum space which is associated with a hidden chiral symmetry will lead to the zero-energy flat band of a zigzag nanoribbon and some anomalous transport properties. Here it is proposed that the Adler–Bell–Jackiw chiral anomaly or non-conservation of chiral charges of Dirac fermions at different valleys can be realized in a confined ribbon of finite width, even in the absence of a magnetic field. In the laterally diffusive regime, the finite-size correction to conductivity is always positive and is inversely proportional to the square of the lateral dimension $W$, which is different from the finite-size correction inversely proportional to $W$ from the boundary modes. This anomalous finite-size conductivity reveals the signature of the chiral anomaly in graphene, and it is measurable experimentally. This finding provides an alternative platform to explore the purely quantum mechanical effect in graphene.

1. Introduction

Graphene [1] is a monolayer of carbon atoms packed into a hexagon lattice to host spin degenerate two-dimensional Dirac fermions. Each kind of Dirac fermion has two Dirac cones with opposite chirality, where the well-defined Berry phase $\pi$ or $-\pi$ rests [2–5]. The chiral nature and topological properties of the Dirac fermions in graphene have been extensively discussed over the past decade, such as the anomalous integer quantum Hall effect [6, 7] and Klein tunneling [8]. The existence of the flat band of the edge states in a zigzag ribbon has stimulated extensive studies of transport properties in graphene nanoribbons, which has emerged as valley physics [9, 10]. Stimulated by the recent advances in three-dimensional Weyl/Dirac fermions in topological Weyl/Dirac semimetals [11–18], we come to re-examine the topological properties and chiral physics of two-dimensional Dirac fermions in graphene.

From the tight-binding model for electrons in graphene, it was shown that non-zero electric polarization exists in reduced one-dimensional momentum space, which is associated with a hidden chiral symmetry [19]. This topological invariant leads to the famous zero-energy flat band for a stripe of graphene with a zigzag boundary. For a zigzag nanoribbon of finite width, the energy band dispersions become a series of discrete one-dimensional bands, which are very similar to the Landau bands for the Weyl fermions in a magnetic field, and the chiral currents exist along the boundary. Here we propose that the Adler–Bell–Jackiw chiral anomaly [20, 21] or non-conservation of chiral charge at two different valleys, can be realized by applying an electric field along the ribbon. The change rate of chiral electrons at each valley is proportional to the electric field, but inversely proportional to the lateral dimension $W$. In the laterally diffusive regime where the mean free path $l$ is shorter than $W$, the energy balance between two valleys and the Joule’s heating of electric current gives rise to a residual correction, which is inversely proportional to $W^2$, to the finite-size conductivity. This is different to the case where the conductivity is inversely proportional to $W$ if the lateral modes can be resolved or with the mean free path that $l \gg W$. This anomalous behavior of the finite-size effect indicates that a narrower ribbon may have a larger finite-size conductance, manifesting a signature of the chiral anomaly of two-dimensional Dirac fermions in graphene.
2. Spinless graphene as a two-dimensional topological Dirac semimetal

As the spin–orbit coupling in graphene is tiny [22], we assume the spin degeneracy of electrons here. The energy dispersions of electrons in graphene have been investigated extensively [1, 23]. To diagonalize the tight-binding model for graphene, a basis of two-component ‘spinors’ of Bloch states constructed on two sublattices A and B is introduced [1]. Let \( \delta_1, \delta_2 \) and \( \delta_3 \) be the displacements from a B site to its three nearest-neighbor A sites, as shown in figure 1(a). The lattice vectors are chosen to be \( \mathbf{a}_1 = \sqrt{3} a (\frac{\sqrt{3}}{2}, \frac{1}{2}) \) and \( \mathbf{a}_2 = \sqrt{3} a (\frac{\sqrt{3}}{2}, -\frac{1}{2}) \). The corresponding reciprocal lattice vectors are \( \mathbf{b}_1 = \frac{4\pi}{3a} (\frac{1}{2}, \frac{\sqrt{3}}{2}) \) and \( \mathbf{b}_2 = \frac{4\pi}{3a} (\frac{1}{2}, -\frac{\sqrt{3}}{2}) \). In this representation the Hamiltonian becomes

\[
H = -t \sum_k \begin{pmatrix} 0 & \phi(k) \\ \phi^*(k) & 0 \end{pmatrix}
\]

where \( \phi(k) = \sum_{n=1}^{3} e^{ik \cdot \mathbf{a}_n} \phi_n \). The energy band dispersions are obtained as,

\[
E_s = -st |\phi(k)|^2,
\]

where \( s = \pm \). The two bands touch at the points \( \mathbf{k} = (\frac{2\pi}{3a}, \frac{2\pi}{3\sqrt{3}a}) = \frac{1}{2} \mathbf{b}_1 + \frac{2}{3} \mathbf{b}_2 \) and \( \mathbf{k}' = (\frac{2\pi}{3a}, -\frac{2\pi}{3\sqrt{3}a}) = \frac{1}{2} \mathbf{b}_1 + \frac{2}{3} \mathbf{b}_2 \) in the Brillouin zone formed by the reciprocal lattice vectors \( \mathbf{b}_1 \) and \( \mathbf{b}_2 \), as shown in figure 1(b), and the dispersions become linear in \( \delta k = |\mathbf{k} - \mathbf{k}'| \) approximately measured from the two points. Thus two Dirac cones are formed around \( \mathbf{k} \) and \( \mathbf{k}' \). The density of states is linear in energy \( E \) near the two Dirac points, which is a key feature of a semimetal. The vector connecting \( \mathbf{k} \) and \( \mathbf{k}' \) is along \( \delta \mathbf{k} = \mathbf{k} - \mathbf{k}' = \frac{1}{2} (\mathbf{b}_1 - \mathbf{b}_2) \). To explore the topological properties of the two Dirac cones, we take \( \mathbf{k} = k_1 \mathbf{b}_1 + k_2 \mathbf{b}_2 \) and consider a specific direction by taking a specific value of \( k_1 \) (or \( k_2 \)) as a constant, and the model is reduced to be one-dimensional along the \( \mathbf{b}_1 \) (or \( \mathbf{b}_2 \)) direction. When \( k_1 \) is away from the Dirac points, i.e. \( k_1 \geq 1/3 \) and \( 2/3 \), the reduced one-dimensional system always possesses a finite band gap. This gap will close and re-open when \( k_1 \) sweeps over one Dirac point, which indicates that a topological phase transition may occur in the process.

Ryu and Hatsugai [19] first realized that zero energy modes in the zigzag ribbon of graphene are closely associated with a hidden chiral symmetry for a reduced one-dimensional Hamiltonian in a parameter space. Denote the eigenstates of \( H \) by

\[
|\phi(k_x, k_y)\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ s \phi(k) \end{pmatrix}
\]

with the eigenvalue \( E_s(k) \) in equation (2). In the reduced one-dimensional momentum space, e.g. keeping \( k_1 \) constant, the electric polarization for the reduced one-dimensional band is defined as [24, 25]

\[
P(k) = -\frac{e\sqrt{3}a}{2\pi} \oint C dk \langle \phi(k, k_2) | (i\mathbf{\omega}_b) | \phi(k, k_2) \rangle.
\]

The electric polarization has its topological origin, and is quantized to be \( P = e\sqrt{3}a/2 \) where the integer \( \nu = 0 \) or \( 1/2 \) with modulo 1 appears as a topological invariant for quantum transport. It is found that \( P = e\sqrt{3}a/2 \) for \( 1/3 \leq k_1 \leq 2/3 \), and \( P = 0 \) otherwise. Thus the one-dimensional system is topologically nontrivial when \( 1/3 \leq k_1 \leq 2/3 \). Therefore a spinless graphene is a two-dimensional topological Dirac semimetal characterized by a topological invariant, which is very similar to the three-dimensional Weyl semimetal where a \( k \)-dependent Chern number is defined [26]. According to the bulk-boundary correspondence, a pair of end modes exists near the two ends of an open and topological nontrivial chain, and the energy of the end states should be zero due to the chiral symmetry [19], just as in the end modes in the Su–Schrieffer–Heeger model [27]. Correspondingly, the open boundary parallel with the vector \( \mathbf{b}_1 \) (or \( \mathbf{b}_2 \)) is the zigzag boundary of the lattice. Each \( k_1 \) in the shadow regime will have a pair of zero energy modes near two edges according to the the bulk-edge correspondence and the particle-hole symmetry in equation (1), and a flat band is formed for a zigzag boundary of the graphene ribbon. This demonstrates that the famous flat band of graphene with a zigzag boundary condition has its topological origin related to the non-zero electric polarization or topological invariant, just as with the Fermi arc in three-dimensional Weyl semimetals [28]. Unlike a magnetic monopole located at a three-dimensional Weyl node, a well-defined \( \pi \) Berry phase exists around the Dirac point in two dimensions [2–4].

3. Chiral anomaly

It is well known that the chiral charge conservation may be violated for Weyl fermions in three dimensions. Nielsen and Ninomiya [29] proposed to simulate the chiral anomaly in one-dimensional chiral bands by using the lowest Landau band of a three-dimensional semimetal in the presence of a magnetic field. Applying
an external electric field along the magnetic field will drive electrons flowing from one node to another one, which leads to the so-called Adler–Bell–Jackiw chiral anomaly [20, 21]. Consequently, it is expected that the longitudinal magnetoresistivity becomes extremely strong and negative [29]. If the electric field is normal to the magnetic field, the anomaly will disappear. Recently, thanks to the discovery of a number of realistic materials of topological semimetals [16, 17], there is growing interest in their electronic transport and signatures of the chiral anomaly [18, 30–32]. Inspired by the advances in three-dimensional Weyl semimetals, whether or not the chiral anomaly or its signature also exists in a two-dimensional Dirac semimetal or graphene has become an appealing issue [5]. A perpendicular magnetic field can induce discrete Landau bands, but it is always perpendicular to the electric field or electric current in graphene, and an in-plane magnetic field cannot produce Landau bands. Thus it is obvious that there is no chiral anomaly in graphene in the presence of both magnetic and electric fields, in contrast to the three-dimensional case. However, early works on the quasi-one-dimensional graphene nanoribbon have shown that they may support the formation of one-dimensional chiral bands due to the finite-size effect of quantum confinement [33].

Consider a monolayer graphene sheet encapsulated by two confining gates or potentials along the zigzag direction. The shadow area means a confining potential $V(x)$ is added, say $V(x) = V_0|x|$ where $x$ is the position measured from the potential boundary, i.e. the dashed lines. The potential is zero in the white regime. (b) The energy band dispersions near two Dirac points. $k$ is the wave vector. The parameters are $N = 20, V_0 = \frac{a}{\pi}$ and $a_0 = \sqrt{3}a$.

Figure 2. (a) Schematic of a carrier-guiding graphene sheet encapsulated by two confining gates or potentials along the zigzag direction. The shadow area means a confining potential $V(x)$ is added, say $V(x) = V_0|x|$ where $x$ is the position measured away from the dashed line or the potential boundary, or as shown in figure 2(a). $V_0$ represents the strength of the confining potential. It is worth emphasizing that the final result in this paper is not so sensitive to the form of the confining potential as to the effective Fermi velocity of the Dirac fermions which is almost independent of the form of the confining potential. Due to the effect of quantum confinement, the energy dispersion evolves into a set of one-dimensional chiral bands. Modes $n = 1, 2, 3, \cdots, N$ lie in the right valley whereas modes $n = -1, -2, \cdots, -N$ lie in the left valley. At each valley, the energy spacing for different non-zero energy bands is approximately $\Delta = \frac{\pi}{a} \frac{a}{2} \frac{N}{w}$, and the gap between the conduction band and valence band is about $3\Delta$. Within the band gap, the zeroth mode, $n = 0$, with nearly linear dispersion crossing the two Dirac points at $k = \pm 1/3$ with opposite velocities, $v = \pm \frac{3}{2}a/\hbar$. Take the periodic boundary condition along the vertical direction. The energy band dispersion is shown in figure 2(b). The energy dispersions are split into a series of energy bands due to the confining effect of the potential, which are very similar to the Landau bands induced by an external magnetic field in graphene [34], and also those in topological Weyl semimetals [28]. It is noted that the shape and position of the $n = 0$ mode depends on the strength of the potential. The formation of the $n = 0$ mode originates from the non-zero topological invariant, i.e. the quantized electric polarization for a reduced one-dimensional chain, as we calculated in equation (3). The non-zero electric polarization implies the
existence of end states for an open boundary condition according to the bulk-boundary correspondence. Each invariant corresponds to one edge state. For a zigzag ribbon in the absence of the confining potential, the energy eigenvalue of an edge state is always zero due to the particle–hole symmetry, which leads to the flat band. Equivalently, when $V_0 \to \infty$, it is similar to a zigzag nanoribbon in which the modes will be flattened [10, 33]. The non-flat band is generated when the particle–hole symmetry is broken by the confining potential.

In the absence of an external electric field, if the Fermi level is near $E_F = 0$, the effective velocities at the points of the Fermi level are opposite each other—the right one is positive and the left one is negative, indicating the formation of chiral states. Applying an external electric field will drive electrons flowing from one valley to the other. The change rate of the density of charge carriers at one valley $(\delta n/\delta t)$ is $s \frac{\partial n}{\partial t} = \frac{s}{2\pi W} \frac{2e}{a_0} \frac{dk}{dt}$ and $\frac{d}{dt} \left( \frac{2e}{a_0} \right) = \frac{e}{h}$. Thus the change rate at each valley is

$$\frac{dn}{dt} = \frac{s}{\hbar W} \frac{e E}{h}$$

indicating the violation of the charge conservation at each valley, although the total charge of the whole system is conserved, $\frac{d (n_+ + n_-)}{dt} = 0$. Thus the chiral anomaly of quasi-two-dimensional Dirac fermions can also be realized as an analog of three-dimensional Weyl fermions in parallel electric and magnetic fields [29]. For three-dimensional Weyl fermions, the changing rate of density at each valley is proportional to $B \cdot E$ ($B$ is the magnetic field and $E$ is the electric field), and the chiral anomaly disappears when the electric field is normal to the magnetic field. Here the anisotropy of the chiral anomaly in graphene is determined by the orientation of the confining potential. If the confining potential is along the armchair direction $a_0$, i.e. along the direction of $a_1 + a_2$, the chiral band crossing the conduction and valence bands may disappear, and consequently, so does the chiral anomaly. For a specific orientation of confining potential between the armchair and zigzag orientation, $a = \cos \theta a_2 + \sin \theta a_0$, where $\theta$ varies from $0$ to $\pi/2$, the change rate will be modified by a factor $\cos \theta$, which approaches zero when $\theta = \pi/2$.

4. Signature of chiral anomaly

Now we come to explore the measurable signature of the chiral anomaly in graphene. It is known that the chiral anomaly of Weyl fermions generates a chiral magnetic effect [29, 35, 36]. Its magnetoconductivity is positive and quadratic in magnetic field $B$ [32]. As the change rate of Dirac fermions at each valley in graphene is proportional to $1/W$, a finite-size conductivity is expected to reveal a signature of a chiral anomaly for Dirac fermions in graphene. Consider the relation between the density of charge carriers $n_\pm$ and the chemical potential $\mu_\pm$, $n_\pm = \frac{1}{4e} \frac{\mu_\pm^2}{(\sigma \tau)^2}$ at each valley. Without loss of generality, assume the chemical potentials are positive, i.e. as in the electron doped case shown in figure 3. In the presence of an electric field, electrons will flow from the right valley to the left valley, and cause a difference of chemical potentials, $\delta \mu = \mu_+ - \mu_-$. However, the process will be balanced by the inter-valley scattering between the left and right moving electrons. Consider the lateral diffusive regime where the mean free path is shorter than the width, and denote the inter-valley scattering time by $\tau_\text{sc}$. The equation for the chiral anomaly is reduced to
\[
\frac{dn_+ - n_-}{dt} = -2 \frac{eE}{hW} n_+ - n_- \tau_v.
\]

In a steady state, the solution to the equation is \(n_+ - n_- = 2 \frac{eE}{hW} \tau_v\). Thus the difference of the chemical potentials at the two valleys is

\[
\delta \mu = \frac{2 \pi \nu (h/\mu)^2}{\nu} \frac{2eE}{hW} \tau_v
\]

(assume \(\mu \neq 0\)). As the Fermi levels at the two valleys are different, and the change rate of electrons is finite due to the chiral anomaly, the energy cost for transferring the electrons from one valley to the other is simply the product of the change rate of electrons at each valley and the energy difference between the two valleys. This energy must be extracted from the Joule’s heating in the presence of a charge current, and the energy balance gives \(\delta E = 2 \frac{eE}{hW} \delta \mu\) [29], where factor 2 comes from the spin degeneracy in graphene. The current is proportional to the difference of the chemical potentials,

\[
\eta = \frac{2e}{hW} \delta \mu.
\]

This formula is similar to that of the chiral magnetic effect if \(I/W\) is replaced by a magnetic field \(B\). Combining with \(\delta \mu\) from the chiral anomaly, the solution to the current is

\[
\eta = \frac{2 e^2 \nu (h/\mu)^2}{\pi \mu W^2} E.
\]

Consequently the conductivity correction due to the chiral anomaly is \(\sigma_W = 2 e^2 \nu (h/\mu)^2 W^2\), which is proportional to \(1/W^2\). It is an anomalous behavior that the conductivity correction increases by decreasing the width in \(W^2\).

The inter-valley scattering time \(\tau_v\) depends on the scattering mechanism. If the scattering potential is short ranged of the form \(V = \nu \delta(r)\), the inter-valley scattering time is given by \(\tau_v \sim \frac{4n_i}{\nu \rho_{\text{Si}}^2} \frac{1}{\rho_{\text{Si}}^2}\) where \(n_i\) is the impurity density [37]. Thus \(\sigma_W\) is proportional to the square root of the density of charge carriers, \(\sigma_W \propto 1/\sqrt{\rho}\). To estimate the order of the finite size correction, we take \(\mu = \tilde{\mu} V, W = W \text{ nm, } I = \nu \tau_v = \tilde{I} \text{ nm, and } \nu = 10^6 \text{ m s}^{-1}\), and have \(\sigma_W \approx 2.63 \frac{\tilde{I}^2 \tilde{\mu}}{\rho W^2 n}\), \(\tilde{\mu} \sim 0.1\) for the charge density \(n \sim 10^{22} \text{ cm}^{-2}\). The inter-valley scattering length is much longer than the mean free path in graphene [37, 38]. Thus for a sample with a scattering length of \(\tilde{I} = 100\), the correction is \(0.263 \frac{\tilde{I}^2}{n}\) for \(W = 100 \text{ nm, which is expected to be measurable experimentally.}\)

\(3\) For \(\mu = 0, \delta \mu = 2 \nu \delta (h/\mu)^2 \tau_v\), and the charge current is

\[
\eta = \frac{2 e^2 \nu (h/\mu)^2}{\pi \mu W^2} E.
\]

However at this point other effects, such as disorders or fluctuations, become dominant to produce a minimal conductivity.

The conventional Drude conductivity of graphene \(\sigma_0\) was found to proportional to the density of charge carriers, \(n\), which reaches a minimal conductivity at the charge neutral point [37, 39–41]. The conductivity is always of the order of \(e^2/\hbar\) and has a weak dependence on size [1, 42]. The quantized conductance in the steps of \(4e^2/\hbar\) has been measured in a graphene nanoribbon [43]. For wires or ribbons without boundary modes, the conductivity usually has a negative correction due to excess scattering from the boundary which is inversely proportional to \(W\). In the presence of a boundary mode, the correction can become positive, but is still inversely proportional to \(W\). However, the anomalous correction here is always positive and is inversely proportional to the square of \(W\).

It is worth emphasizing that the chiral anomaly we discuss here can be regarded as one of the quasi-one-dimensional Dirac fermions in which the charge transfer rating is only proportional to an electric field [44]. This mechanism will generate an imbalance of the chemical potentials \(\delta \mu\) at the two valleys. The result in equation (8) shows that the current density is proportional to \(\delta \mu\), which is similar to the chiral magnetic effect in three dimensions [32]. The negative magnetoresistance in three-dimensional Weyl semimetals is usually associated with this effect. It is noted that a negative magnetoresistance appears even in the absence of a chiral anomaly [45]. Thus the mechanism of the anomalous transport here may be generalized to other two-dimensional materials with valleys.

### 5. Summary

In short, we propose that the chiral anomaly of two-dimensional Dirac fermions can be realized in a quasi-one-dimensional monolayer graphene, and its signature can be detected by measuring the finite-size conductivity. It is necessary to emphasize that we consider the laterally diffusive regime where the mean free path is shorter than the width. When the mean free path is much larger than the width \(W\), the story will be very different. It is believed that this property is associated with the chiral symmetry of the Dirac fermions in reduced one-dimensional momentum space and the formation of chiral currents of the system. The chiral anomaly is a purely quantum mechanical effect for Weyl fermions. It is widely accepted that the positive magnetoconductivity or negative magnetoresistance in topological Weyl semimetals is a signature of the chiral anomaly. The anomalous finite-size conductivity in graphene may provide an alternative way to detect this quantum mechanical effect in solids.

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