Quantum Hall effect in graphene with twisted bilayer stripe defects

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We analyze the quantum Hall effect in single layer graphene with bilayer stripe defects. Such defects are often encountered at steps in the substrate of graphene grown on silicon carbide. We show that AB or AA stacked bilayer stripes result in large Hall conductivity fluctuations that destroy the quantum Hall plateaux. The fluctuations are a result of the coupling of edge states at opposite edges through currents traversing the stripe. Upon rotation of the second layer with respect to the continuous monolayer (a twisted-bilayer stripe defect), such currents decouple from the extended edge states and develop into long-lived discrete quasibound states circulating around the perimeter of the stripe. Backscattering of edge modes then occurs only at precise resonant energies, and hence the quantum Hall plateaux are recovered as twist angle grows.

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I. INTRODUCTION

The unique half-integer quantum Hall effect (QHE) in monolayer graphene serves as a fingerprint of massless Dirac electrons.1,2 It is therefore used in the laboratory to distinguish monolayers from multilayers.3 The electrons in graphene under applied perpendicular magnetic field have an unconventional Landau level spectrum, leading to a sequence of Hall conductivity plateaux $\sigma_{xy} = G_0(2n + 1)$, where $G_0$ is the conductance quantum, $G_0 = 2e^2/h$ ($h$ is Planck’s constant and $e$ is the electron charge), and $n$ is an integer including zero.4

The large energy level separation between the $n = 0$ and $n = 1$ Landau levels adds robustness to the $n = 0$ plateau, which has been observed also at room temperature.5 More importantly, measurements6–8 of the von Klitzing constant $R_K = h/e^2$ have been performed to metrological accuracy on epitaxial graphene on silicon-carbide (SiC). Large breakdown currents have been observed for this material, and epitaxial graphene at present outperforms conventional two-dimensional electron gases in semiconducting heterostructures in this respect, and may very well be the material of choice for metrology in the future. Transistors with promising high cutoff frequencies have also been fabricated from epitaxial graphene.9,10 It is therefore of high current interest to establish the electron transport properties of graphene on SiC.11

Inhomogeneities in the two-dimensional material are often detrimental to its transport properties.12–16 Epitaxial graphene on SiC may continuously cover the whole SiC substrate,17–19 but steps on the substrate influence the graphene layer along lines running across the wafer.20,21 At a step, the graphene sheet may be more decoupled from the underlying substrate than on the wide terraces between steps, which may change the doping level locally.20,22 Graphene may also suffer strain23 since the SiC step is atomically sharp, while the graphene sheet forms a continuous cover. In addition, since the steps serve as seeds in the growth process of epitaxial graphene, bilayers or multilayers are often observed.18,24,25 See Fig. 1(a). Depending on the growth process, several islands may form near the steps or continuous stripes may be formed along a large part of the step. After fabrication of the Hall bar, the bilayer stripe defects can reach from one side to the other of the Hall bar, resulting in a geometry similar to the one shown in Fig. 1(b). Experimentally, it was recently observed26 that narrow Hall bars intentionally fabricated perpendicular or parallel to steps display markedly different properties. When the current path crosses many steps, a positive magnetoresistance arises that can be explained, according to Schumann et al.,26 as the result of Hall edge channel backscattering caused by new edge channels developing along the substrate steps, although the specific mechanism remains an open question.

II. HALL EFFECT ACROSS A TWISTED BILAYER

The properties of bilayer graphene, particularly of twisted bilayers, have been the focus of considerable interest recently.29–32 For $AB$-stacked bilayer graphene, the two Dirac...
cones of a decoupled double monolayer system are strongly modified by the interlayer hopping, resulting in parabolic bands and possibly trigonal warping. In twisted graphene, on the other hand, the two cones within each valley are separated in reciprocal space and interlayer coupling leads to a finite energy saddle point in the band structure at the intersection of the two surviving Dirac cones. The corresponding van Hove singularity has been observed experimentally. The question arises as to what the QHE looks like across a monolayer-bilayer graphene junction, including the effect of interlayer twist in the bilayer part.

It should be recognized that a heterostructure consisting of monolayer graphene occupying the half space \( x < 0 \) and bilayer graphene occupying the other half space \( x > 0 \) is rather different from the geometry considered in this paper, where the bilayer exists between \( 0 < x < L \), see Fig. 1, and plays the role of a complicated barrier for electron flow in the lower extended monolayer. The finite length \( L \) of the bilayer patch leads to the formation of a spectrum with quasibound state resonances. Such states are chiral and circulate around the bilayer.

A. Model

To illustrate the resonant backscattering effect, we have performed quantum transport calculations for two-terminal and six-terminal nanoribbon devices in a magnetic field. We ignore the effects of inhomogenous doping and strain, which may also modify magnetotransport as studied elsewhere, and concentrate on the effect of a bilayer patch. The starting point is the tight-binding Hamiltonian for graphene

\[
H = \sum_{ij} t_{ij} c_i^\dagger c_j,
\]

where the hopping elements \( t_{ij} \) include hopping beyond nearest neighbors, and are modeled by the \( \pi \)-orbital overlap at different carbon sites \( j \) and \( i \) separated by \( \mathbf{R}_j - \mathbf{R}_i = \mathbf{r} = (x,y,z)^T \).

\[
t_{ij} = t(\mathbf{r}) = -\gamma_0 \frac{x^2 + y^2}{r^2} e^{-\gamma_1 |r| - a_{cc}} - \gamma_1 \frac{z^2}{r^2} e^{-\gamma_2 |r| - d}.
\]

Here, \( \gamma_0 \) and \( \gamma_1 = 0.14\gamma_0 \) are the nearest neighbor and interlayer hopping parameters of graphite, \( a_{cc} \) is the carbon-carbon distance in plane, and \( d = 2.4a_{cc} \) is the interlayer distance. The exponent is \( \gamma = 3/\lambda a_{cc} \). The formula in Eq. (2) is applied for atomic distances \( r = |\mathbf{r}| \) reaching a cutoff \( R_c \), beyond which \( t_{ij} = 0 \). This generalization beyond simple nearest-neighbor models is crucial to properly recover the low energy electronic structure of twisted bilayers, in particular its gapless and valley-decoupled double-cone spectrum, as described by the continuum theory of Ref. 29. In practice, a rather precise description at relevant energy scales is obtained for \( R_c \gtrsim 7a_{cc} \).

B. Band structure of the leads

The band structure of the monolayer graphene nanoribbon leads converges rapidly with increasing hopping cutoff \( R_c \), and is shown for a 10 nm wide zigzag nanoribbon with \( R_c = 3a_{cc} \) in Fig. 2 for varying magnetic fields. The magnetic field is included in the model through a standard Peierls’s substitution. We note that, for large \( R_c \), a large unit cell of length \( a_u \gtrsim R_c \) is needed for which the first Brillouin zone in reciprocal space is small. This correlates with the folding of the bands of a nearest neighbor tight-binding model, but leads to slightly more complicated bands due to the long range hoppings; see Fig. 2. For instance, for small magnetic fields, Fig. 2(a), we see a positive energy shift of the cones of about 0.3\( \gamma_0 \) and the zero-energy edge modes of the zigzag ribbon display substantial dispersion. For small magnetic fields \( B \) the magnetic length \( \ell_B = \sqrt{\hbar v_f/|eB|} \) is larger or comparable to the ribbon width \( W \) and the spectrum is dominated by size quantization. This is the case in Fig. 2(a) where the energy split of the zero mode is due to the small magnetic field corresponding to a flux \( \Phi = 10^{-3}\Phi_0 \) per hexagon, where \( \Phi_0 = h/2e \) is the magnetic flux quantum. For larger fields, the Landau levels \( E_n = \sqrt{2n\hbar v_f/\ell_B} = \sqrt{n\omega_c} \) \( (v_f \) is the Dirac electron velocity in the absence of magnetic field) become visible as flat regions in the dispersion. The dispersive parts of
the bands correspond to edge modes, carrying the current in the quantum Hall regime.

III. MAGNETOTRANSPORT SIMULATION

To evaluate the effect of the bilayer patch, we compute magnetotransport properties using recursive Green’s function (RGF) techniques, where the coupling to reservoirs are included through self-energies derived from the surface Green’s functions of semi-infinite leads. The leads and the system are modeled on equal footing through the Hamiltonian in Eq. (1). The RGF algorithm gives the retarded Green’s function of the system. Such Green’s function is obtained, between certain pairs of points, by iterative application of the Dyson equation, and may be then used to compute the Hall conductivity, the current densities, or the scattering matrix of the system. The recursive iteration is performed on slices of the lattice that are connected only to neighboring slices, and which hence increase in size as the hopping cutoff \( R_c \) increases. This has a rather steep computational cost, but has the advantage that it cleanly avoids fermion doubling problems that plague strategies based on the discretization of low energy effective theories in graphene, and can moreover quantitatively incorporate the precise edge termination of each of the Hall bar regions.

A. Multiterminal Hall conductivity

In Fig. 3 we display a six-terminal monolayer graphene Hall bar device with six contacts (leads) enumerated by L1–L6. In a typical experiment, a current is sent from L1 to L2, and the voltage between L3 and L5 gives the longitudinal resistance, while the Hall resistance is obtained by measuring the transverse voltage between, for instance, L5 and L6. Since this Hall bar is of monolayer graphene only, it is sufficient to use a nearest neighbor model. After computation of the full scattering matrix connecting the six leads, we compute the longitudinal resistance \( \rho_{xx} \) and the transverse conductance \( \sigma_{xy} \) in the linear response regime. We display both in Fig. 3(c) as a function of Fermi energy of the system (related to the electron density). The transverse conductance display quantized values \( \sigma_{xy} = \pm (2n + 1) G_0 \), where \( G_0 = 2e^2/h \) and \( n = 0, 1, 2, \ldots \). This sequence is characteristic for the monolayer quantum Hall
and the transverse conductance $\sigma_{xy}$ to a flux and L1 with respect to the other leads. The applied field corresponds the two edges at stacked bilayer stripe defect in the middle of the device, connecting G and L6 (green squares). The color scale in (a) is given in units of measured either between L5 and L6 (black squares) or between L3 and L6 (green squares). The color scale in (a) is given in units of the longitudinal resistance $\rho_{xx}$ and the transverse conductance $\sigma_{xy}$, computed for a voltage measured either between L5 and L6 (black squares) or between L3 and L6 (green squares). The color scale in (a) is given in units of $G_0 V$, where $V$ is the small increase of the chemical potentials in L6 and L1 with respect to the other leads. The applied field corresponds to a flux $\Phi = 0.01\Phi_0$ per hexagon, and the temperature is zero.

![Image](image_url)

**FIG. 4.** (Color online) (a) Hall bar with a $L = 10$ nm long AB-stacked bilayer stripe defect in the middle of the device, connecting the two edges at $y = 0$ and $y = 20$ nm. The local current flow pattern is for the Fermi energy $E_F = 0.5\gamma_0$ [the same as in Fig. 3(a)]. (b) The longitudinal resistance $\rho_{xx}$ (red dots; voltage measured between L3 and L5) and the transverse conductance $\sigma_{xy}$, computed for a voltage measured either between L5 and L6 (black squares) or between L3 and L6 (green squares). The color scale in (a) is given in units of $G_0 V$, where $V$ is the small increase of the chemical potentials in L6 and L1 with respect to the other leads. The applied field corresponds to a flux $\Phi = 0.01\Phi_0$ per hexagon, and the temperature is zero.

effect. The longitudinal resistance is zero except at the steps between plateaux. The random fluctuations at the steps are due to the added randomness of 10% of the nearest neighbor hopping integral $t_{ij}$ around $\gamma_0$ in this simulation.

The current flows along edge states, as is clearly seen in Fig. 3(a), which shows the local current flow patterns throughout the device when currents are injected at L6 and L1 and subsequently collected at L4 and L3. In Fig. 3(b) we show the current redistribution throughout the entire device that appears at each step between plateaux (in this case the $n = 1$ and $n = 2$ plateaux at $E_F = 0.4507\gamma_0$).

In Fig. 4 we show the influence of an AB-stacked bilayer stripe defect placed in the middle and connecting the two edges of the Hall bar. The current can now enter into a circular path around the bilayer patch and eventually go out into both leads L5 and L4; see Fig. 4(a). This leads to large fluctuations of the longitudinal resistance $\rho_{xx}$, as shown in Fig. 4(b), red circles. At the same time, the transverse conductance is affected. If the voltage probes are set between L5 and L6, the influence of the patch is minimal. On the other hand, when the voltage probes span the patch, for instance when they are placed between L3 and L6, the fluctuations are added into $\sigma_{xy}$ as well, and the plateaux are destroyed.

**B. Two-terminal conductance and twist angle**

Next we study the influence of a finite twist angle on the fluctuations of the Hall conductance. In contrast to the AB-stacked bilayer patch explored above, this requires that we include long-range hopping $t_{ij}$ with a cutoff $R_c = 7a_{cc}$. For this study it is convenient to limit the calculations to a two-terminal setup, as in Fig. 1(b). In the absence of contact resistances, like in the present case, the two-terminal conductance equals the Hall conductivity $\sigma_{xy}$. In Fig. 5 we show the conductance for a $W = 10$ nm wide ribbon in a quantizing magnetic field as function of Fermi energy (i.e., doping). The band structure of the underlaying monolayer is shown in Fig. 2(d). The bilayer patch length is $L = 10$ nm. The twist angle $\theta = 0$ corresponds to a bilayer patch with AB stacking, while $\theta = 60^\circ$ would correspond to AA stacking. For small twist angles, all plateaux are destroyed by backscattering caused by a number of resonance states in the patch, which are rather broad and tend to overlap. For increasing twist angle, these resonances become sharper, signaling a decoupling of the quasi bound states from the edge modes in the underlying monolayer that is connected to source and drain reservoirs. The plateaux become better defined, starting with the $n = 0$ plateau at small twist angle and continuing with the higher Landau level index plateaux at higher twist angles (higher index require larger twist angle to recover).

The dependence with twist angle of the width of the backscattering resonances, or, in other words, of the...
coupling between the corresponding quasibound state and the monolayer edge states, can be traced to the band structure of the twisted bilayer. In the limit of a vanishing interlayer coupling $\gamma_1 \ll \gamma_0$, the states become perfectly bound and lie fully on the decoupled layer. Their momentum components are concentrated around the Dirac point of said layer. In contrast, the delocalized edge states in the extended monolayer are spectrally concentrated around the monolayer Dirac point, which has a shift $\Delta K = 2 \sin(\theta/2) \times 4\pi/(3\sqrt{3}a_c)$ [for $0 < \theta < 30^\circ$] with respect to the former. The momentum spread grows linearly with energy. Therefore, for a given energy, the larger the momentum mismatch of the two Dirac points, the smaller the overlap between delocalized edge states and localized patch states will be. Since this overlap is a measure of the inverse lifetime of the quasibound state in the limit of small $\gamma_1/\gamma_0$, we see that twist angles around 30° (halfway between AB and AA stacking, maximum $\Delta K$) will correspond to least coupling, narrower resonances, and cleaner Hall plateaux, as seen in Fig. 5.

A second consequence of this analysis is that, as soon as the Fermi energy approaches the van Hove singularity where the two Dirac cones intersect (at energy $\sim v_F \Delta K/(2 - \gamma_1)$), the spectral spread becomes comparable to $\Delta K$, so the overlap will increase greatly, and the backscattering will be enhanced. Hence higher Hall plateaux will be eventually destroyed for any value of the twist angle as the filling factor grows. This is also apparent in Fig. 5(a). For instance, for $\theta = 20^\circ$ (blue curve), it is clear that the $n = 0$ and $n = 1$ plateaux have sharp resonances, while plateau $n = 2$ and especially plateaux $n \geq 3$ at higher doping (i.e., higher $E/\gamma_0$) are destroyed.

C. Circulating quasibound states

To demonstrate the connection between resonant backscattering and quasibound states of circulating currents around the patch, we present in Fig. 6 the local current flow pattern throughout the system for filling factors near and at the resonance dip indicated by the blue arrow in Fig. 5(b). In the first panel the edge current flows from left to right, from source to drain, along the upper edge in the $n = 0$ Landau level of the monolayer undisturbed by the patch. On resonance (fourth panel) the current circulates in the patch and suffers perfect back reflection at the lower edge (blue back-flowing current), and the conductance from such edge state is zero on resonance. Similar resonances occur at higher plateaux, where resonant backscattering from each patch state always removes at most one conductance quantum $G_0$ from the Hall conductivity (assuming unbroken spin symmetry).

D. Effects of disorder

In the above two-terminal simulations of the bilayer stripe defect we have neglected disorder. A simple model of disorder was included in the six-terminal simulations in Sec. III A through a 10% randomization of the nearest neighbor hopping integrals $t_{ij}$ around $\gamma_0$ in that case. To simulate the influence of disorder on the conductance fluctuations induced by the bilayer patch, we do the same for the $t_{ij}$ in Eq. (2). In practice, we make the substitution $t_{ij} \rightarrow t_{ij}(1 + \lambda \rho_{ij})$, where the level of disorder is $\lambda$ and $\rho_{ij}$ is a random number between $-0.5$ and $0.5$. In Fig. 7 we show results of this type of disorder for a bilayer patch with twist angle $\theta = 20^\circ$ for energies $E \in [0.63, 0.66] \gamma_0$, which is on the $n = 1$ plateau in Fig. 5. We vary the disorder strength from $\lambda = 5\%$ to $\lambda = 30\%$, with the same random number sequence $\rho_{ij}$. For small disorder strength, the resonances are shifted in energy. For increasing disorder strength (bigger $\lambda$), resonances get broadened. Eventually, resonances overlap and the plateau is completely destroyed again, despite its $\theta = 20^\circ$ twist angle. This destruction can be understood as due to enhanced momentum relaxation that reduces the effect of the momentum mismatch between the Dirac cones of the two

![Image](544x582 to 550x649)

![Image](544x664 to 550x732)
layers that in the first place (without disorder) decoupled the layers and lead to sharp resonances. We find, thus, that a sizable amount of disorder is necessary to cause an appreciable correction to the general results found in the clean case.

IV. CONCLUSIONS AND OUTLOOK

We have analyzed the effect of bilayer stripes transverse to graphene Hall bars on the Hall conductivity. Such stripes are observed to naturally arise at substrate steps in epitaxially grown graphene. We have found that, in agreement with Ref. 26, the Hall plateaux are destroyed by the coupling between opposite edge states via transverse transport channels circulating around the bilayer perimeter. Such channels arise as a result of the jump in Chern number between the band structures of bilayer and monolayer graphene, and give rise to the formation of circulating quasibound states in finite length bilayer patches. Hall plateaux develop backscattering to the formation of circulating quasibound states in finite structures of bilayer and monolayer graphene, and give rise as a result of the jump in Chern number between the band period of the twisted bilayer patch $L_M = \sqrt{3a_{cc}}/2 \sin(\theta/2)$.

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QUANTUM HALL EFFECT IN GRAPHENE WITH TWISTED...

PHYSICAL REVIEW B 87, 205429 (2013)

36M. Z. Hasan and C. L. Kane, Rev. Mod. Phys. 82, 3045 (2010).
41Note that the peak in Fig. 5 around 0.25γ0 (in the zeroth plateau), is related to the dispersive zero mode characteristic of the zigzag nanoribbon of Fig. 2(d).