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The effect of spin mixing on the quantum Hall effect in graphene

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Abstract
On the basis of a tight-binding model, we study numerically the effect of Rashba spin–orbit coupling on the quantum Hall effect in graphene. It is found that the spin–orbit coupling can open a gap in the energy spectrum of the counterpropagating edge states in the $\nu = 0$ plateau region, while the edge states in other plateau regions remain gapless. In the presence of disorder, the energy spectrum in the $\nu = 0$ plateau region shows the feature of level repulsion, an indication of switching on of backward scattering and localization of the edge states. This result may explain the insulator-like behavior near the Dirac points observed in experiments at low temperatures.

(Some figures in this article are in colour only in the electronic version)

Recently, the novel transport properties of the Dirac-like electrons in graphene, a single-atom-thick film of carbon atoms densely packed in a honeycomb lattice, have become the major focus of many research activities, since this new two-dimensional material was successfully fabricated [1, 2]. Graphene is promising for electronic device applications because of the high mobility, easy control of carrier densities, and many other attractive characteristics. The anomalous quantum Hall effect (QHE) is one of the exotic transport properties of graphene subjected to intensive experimental and theoretical study [3–17].

In a relatively weak magnetic field, where the Zeeman splitting is negligible, the Hall conductivity of graphene takes the form $\sigma_{xy} = \nu\frac{e^2}{\hbar}$ with $\nu = (k + \frac{1}{2})g_s = \pm 2, \pm 6, \ldots$, where k is an integer, and $g_s = 4$ accounts for the spin and sublattice-related Dirac valley degeneracies of the Landau levels. This interesting 'half-integer' quantization rule was observed experimentally [3, 4], and explained theoretically [5–9] as resulting from the Berry phase anomaly at the Dirac points [18]. In a strong magnetic field, where the Zeeman splitting is strong enough to lift the spin degeneracy, all even-integer $\nu = 2k$ Hall plateaus become possible in principle, as illustrated in figures 1(a)–(c). In recent experiments, by using ultra-high magnetic fields [10], the additional Hall plateaus $\nu = \pm 4$ caused by the Zeeman splitting were observed. Interestingly, extra odd-integer $\nu = \pm 1$ Hall plateaus also appeared in the experiments [10], which have been attributed to spontaneous valley symmetry breaking driven by the electron–electron interaction [11–17].

If the two spin degrees of freedom are decoupled, a $\nu = 0$ plateau will appear near the Dirac points. This plateau state is topologically distinct from an ordinary insulator state, as it is a superposition of the $\nu = 1$ plateau state of the spin-up electrons and the $\nu = -1$ plateau state of the spin-down electrons, as seen from figures 1(a)–(c). Correspondingly, for a sample with an open boundary, there are two gapless conducting edge modes with opposite spin polarizations in the $\nu = 0$ bulk gap, counterpropagating on each edge of the sample [19], as sketched in figure 1(d). For comparison, the edge states in the $\nu = 2$ and 4 bulk gaps are shown in figures 1(e) and (f), where the edge states for different spins are moving in the same direction on each edge. When the electron Fermi energy lies in the $\nu = 0$ bulk gap, the system is expected to show hallmarks of the standard QHE. On the experimental side, however, the Hall effect near the Dirac points are found to be quite unusual. Abanin *et al* [20] observed that the longitudinal resistivity ρ_{xx} shows a pronounced peak near $\nu = 0$ with magnitude $\rho_{xx} \gtrsim h/e^2$ at temperature $T = 4$ K, in contrast to the standard QHE, where the longitudinal resistivity tends to zero. Phenomenologically, they attributed the large resistivity to dissipative transport of the edge states [20]. Checkelsky, Li and Ong [21] observed that the longitudinal resistivity near

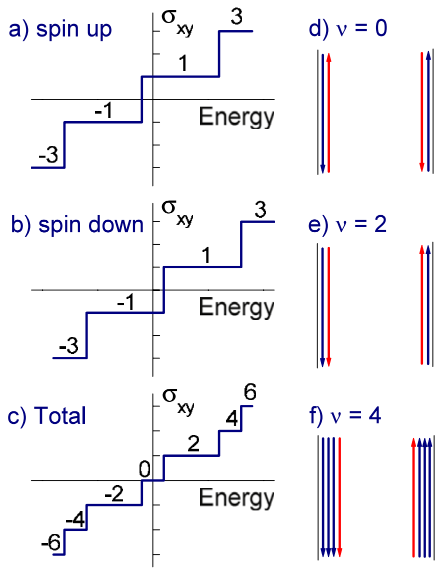

Figure 1. Illustration of QHE and edge states. (a) Hall conductivity for spin-up electrons, (b) Hall conductivity for spin-down electrons, and (c) total Hall conductivity. The Hall plateaus of the opposite spins are shifted relatively due to Zeeman splitting. (d)–(f) Edge states with spin-up (blue lines) and spin-down (red lines) polarizations in the $\nu = 0$, 2 and 4 bulk energy gaps, respectively, where arrows indicate the moving directions of the edge states.

$\nu = 0$ displays a strong divergent trend, by decreasing the temperature down to 0.3 K. These controversies stress the importance of further studying theoretically the unusual nature of the $\nu = 0$ Hall effect, especially its characteristics in the presence of small perturbation of the spin mixing and disorder scattering.

In this paper, we show that the spin-flip effect can inherently destabilize the edge states in the $\nu = 0$ bulk energy gap, leading to insulating behavior near $\nu = 0$. While the spin-flip scattering in graphene is relatively weak, it is still an observable effect, as suggested by the spin precession experiment [22]. We study numerically the effect of Rashba spin–orbit coupling, as an exemplary spin-flip perturbation, on the QHE in graphene. It is found that the spin–orbit coupling can open a gap in the energy spectrum of the counterpropagating edge states in the $\nu = 0$ bulk gap, while the parallel-moving edge states in other plateau regions remain gapless. In the presence of disorder, the edge-state spectrum in the $\nu = 0$ bulk gap exhibits level repulsion behavior, indicating the switching on of backward scattering and localization of the edge states. This finding may explain the insulator-like behavior near the Dirac points observed in experiments.

We consider a rectangular graphene sample with two armchair edges and two zigzag edges. The y-axis is chosen to be parallel to the armchair edges and the x-axis parallel to the zigzag edges. The sample size is denoted by $L_x \times L_y$, where L_y is the number of zigzag chains, and L_x is the number of atoms on each zigzag chain. A magnetic field is applied perpendicular to the graphene plane. The tight-binding model Hamiltonian for the system is written as

$$H = -t\sum_{\langle ij\rangle} \mathrm{e}^{\mathrm{i}\varphi_{ij}} c_i^\dagger c_j - \frac{g}{2}\sum_i c_i^\dagger \sigma_z c_i + \mathrm{i}V_{\mathrm{R}}\sum_{\langle ij\rangle} c_i^\dagger \hat{\mathbf{e}}_z \cdot (\boldsymbol{\sigma}\times\mathbf{d}_{ij})c_j + \sum_i w_i c_i^\dagger c_i, \quad (1)$$

where $c_i^\dagger = (c_{i\uparrow}^\dagger, c_{i\downarrow}^\dagger)$ are the electron creation operators, and $\boldsymbol{\sigma}$ are the Pauli matrices. The first term is the nearest-neighbor hopping term with φ_{ij} a phase factor acquired by an electron moving in the magnetic field. $\sum_{\bigcirc}\varphi_{ij} = \frac{2\pi}{M}$ is the magnetic flux per hexagon in units of the flux quantum $\phi_0 = \frac{hc}{2e}$ with M as an integer. The second term stands for the Zeeman coupling, where g is the Zeeman splitting between the opposite spins. The third term is the Rashba spin–orbit coupling, where $\hat{\mathbf{e}}_z$ is a unit vector along the z direction (vertical to the graphene plane), and $\mathbf{d}_{ij}$ is a vector pointing from site j to i. For graphene, the spin–orbit coupling can originate from the undulating surface as well as the gate electric voltage [23], the former effect dominating at small gate voltages. The last term is the on-site random potential accounting for nonmagnetic disorder, where w_i is assumed to be uniformly distributed in the range $w_i \in [-W/2, W/2]$.

The Hamiltonian equation (1) is solved numerically by the exact diagonalization method with a periodic boundary condition $\Psi(\mathbf{R}_i + 3L_y a_0\hat{\mathbf{e}}_y/2) = \Psi(\mathbf{R}_i)$ in the y direction, and an open boundary condition in the x direction, where $\Psi(\mathbf{R}_i)$ represents the electron wavefunction at the ith site with coordinates $\mathbf{R}_i$. A Landau gauge that preserves the translational symmetry in the y direction is adopted, such that the longitudinal momentum q_y (in $\hbar = 1$ units) can be used as a good quantum number. The calculated energy spectra for sample size 128×2000 in three different energy regions are shown in figures 2(a)–(c). In the $\nu = 4$ Hall plateau region shown in figure 2(a), the two straight horizontal lines are two Landau levels, and the curved lines running up and down are the edge states propagating on the two edges of the graphene strip. There are in total eight edge-state lines connecting up the two Landau levels (noting that $3q_y a_0 = 0$ and 2π are equivalent), yielding eight edge modes, four on either edge of the graphene strip, as illustrated in figure 1(f). We can see that the edge states in the $\nu = 4$ plateau region remain gapless, even though the spin–orbit coupling is nonzero. In the $\nu = 2$ plateau region shown in figure 2(b), the edge states are found to be gapless as well. In the $\nu = 0$ plateau region, however, a small energy gap Δ opens up at zero energy, as shown in figure 2(c). Such an energy gap is caused by the nonvanishing spin–orbit coupling, which does not exist if V_{R} is taken to be zero (see the red lines in the inset of figure 2(c)).

In figure 3(a), the energy gap Δ as a function of the normalized Rashba spin–orbit coupling strength V_{R}/t for different values of Zeeman energy is plotted, where $M = 32$ and the sample size is set to 256×2000. The energy gap increases with V_{R}, roughly in linear proportion for small V_{R}. With increasing Zeeman energy g, the energy gap increases as well. In figure 3(b), the energy gap Δ is plotted as a function of the strip width L_x for two different values of g, where Δ is seen to be almost independent of L_x. Figure 3(c) illustrates the magnetic field dependence of Δ. With increasing M ($1/M$ being proportional to the applied magnetic field), Δ decreases

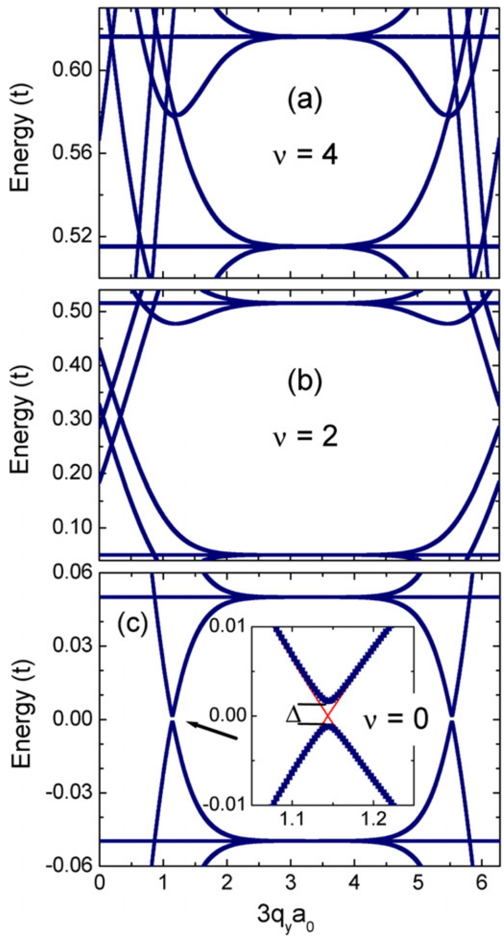

Figure 2. Energy spectrum around the (a) $\nu = 4$, (b) $\nu = 2$ and (c) $\nu = 0$ bulk gaps for a clean sample ($W = 0$) of size 128×2000 with a_0 as the side of the hexagon. Here, the Rashba spin–orbit coupling strength is $V_R = 0.01t$, the magnetic flux parameter $M = 32$, and the Zeeman coupling $g = 0.1t$. The inset in (c) is an enlargement of the energy spectrum around the edge-state energy gap, where thin red lines are the energy spectrum in the absence of spin–orbit coupling ($V_R = 0$).

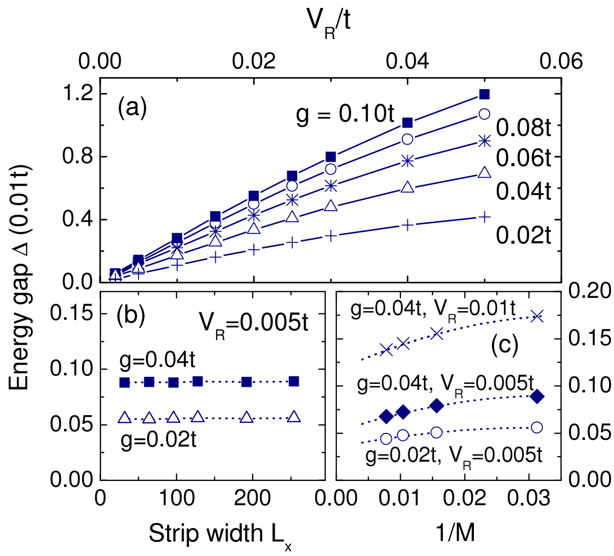

Figure 3. The edge-state energy gap Δ as functions of (a) strength of the Rashba spin–orbit coupling V_R, (b) sample width L_x, and (c) strength of the magnetic flux $1/M$. In (a) and (b), the magnetic flux is fixed at $M = 32$.

slowly. From these results, it follows that the energy gap remains finite no matter whether the strip width becomes very large or the magnetic field tends to be very small. It vanishes only when the Rashba spin–orbit coupling goes to zero.

We further consider the disorder effect on the energy spectrum. The graphene strip under consideration with a periodic boundary condition in the y direction may also be equivalently regarded as a cylinder. A Laughlin gauge experiment [24, 25] can be performed by adiabatically threading a magnetic flux through the cylinder. The magnetic flux in units of the magnetic flux quantum ϕ_0 is denoted as θ_y. In the calculation, the effect of the inserted flux can be easily taken into account by replacing the periodic boundary condition in the y direction with a twisted boundary condition [25] $\Psi(\mathbf{R}_i + 3L_y a_0 \hat{\mathbf{e}}_y/2) = e^{i\theta_y}\Psi(\mathbf{R}_i)$. The calculated electron eigenenergies as functions of θ_y for a sample of size 64×128 in two different regions are shown in figure 4, where for clarity only the edge states on one edge are plotted. Inside the $\nu = 0$ bulk gap in figure 4(a), in the absence of spin–orbit coupling and disorder, the energy levels cross each other, and evolve into different states after a 2π flux is inserted (thin red lines), suggesting that the edge states are conductive. However, when the spin–orbit coupling and disorder scattering are turned on, the energy levels avoid crossing each other (thick blue lines), and return to their original states after a 2π flux is inserted. This level repulsion behavior signals the occurrence of backward scattering and localization of the edge states. It always happens regardless of the disorder strength. On the other hand, inside the $\nu = 2$ plateau region, the energy levels always evolve into different states after a 2π flux is inserted even in the presence of spin–orbit coupling and disorder scattering, as shown in figure 4(b), so the electrons can be continuously pumped from one edge to the other, resulting in the QHE, according to the Laughlin's argument [24].

Our numerical results indicate that the edge states in the $\nu = 0$ plateau region are sensitive to the spin-mixing effect caused by the spin–orbit coupling, in contrast to those in other Hall plateau regions, which are robust against this kind of perturbation. In the presence of disorder, the edge states are Anderson localized, and the system enters a topologically trivial insulating phase, if the electron Fermi energy lies in the $\nu = 0$ bulk gap. For sufficiently pure samples, the localization length of the edge states may be mainly controlled by the spin–orbit coupling [20]. Here, we consider the spin–orbit coupling as originating from the ripples [23]. For typical ripples observed, the Rashba spin–orbit coupling is estimated to be of the order of 0.2 K [23]. Therefore, insulator-like behavior, such as diverging resistivity, should be observable at sufficiently low temperatures, which may explain the divergent trend of the longitudinal resistivity observed at very low temperatures around 0.3 K [21]. On the other hand, due to the smallness of the energy gap in the edge-state spectrum, at relatively high temperatures, dissipative transport through the edge states may

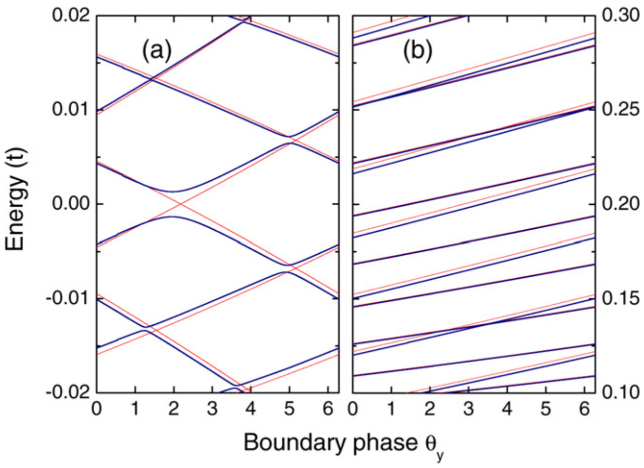

Figure 4. Eigenenergies of the edge states in the (a) $\nu = 0$ and (b) $\nu = 2$ bulk gaps in a sample of size 64×128 for $V_R = W = 0$ (thin red lines) and $V_R = W = 0.01t$ (thick blue lines). The other parameters are taken to be $M = 32$ and $g = 0.1t$, and the disorder configuration is randomly chosen.

become possible, which can greatly reduce the longitudinal resistivity [20].

We wish to point out that the spin–orbit coupling is not the only possible origin of the insulating behavior near $\nu = 0$. For instance, magnetic impurities can also lead to the same behavior. In the present non-interacting model, the Landau level occupation is dominated by the Zeeman coupling. In realistic systems, interactions could potentially modify the $\nu = 0$ ground state, and favor a spin-unpolarized state. In this general case, numerical study would become very difficult and will be left to future works. However, we believe that our conclusion will not change qualitatively, since any spin-flip effect will generally couple the counterpropagating edge states, leading to backward scattering of electrons and thus insulating transport behavior near $\nu = 0$. In this paper, we have confined ourselves to the weak disorder regime. In experiments [21, 26], it is shown that a relatively strong magnetic field is needed in order to observe the insulating behavior around $\nu = 0$. This may be due to relatively strong disorder in the experimental samples, which causes broadening of the Landau levels. As a result, a strong magnetic field is needed to provide good separation of the neighboring Landau levels around $\nu = 0$ and for observing the insulating behavior. However, disorder alone does not explain the insulating behavior, since without spin mixing, the edge states for a given spin are chiral and cannot be localized. We expect that, for samples with higher mobilities, the insulating behavior around $\nu = 0$ will appear at weaker magnetic fields.

In summary, we have numerically investigated the edge-state spectrum of graphene in the presence of spin–orbit coupling and disorder. It is found that the energy spectrum of the edge states in the $\nu = 0$ plateau region opens a small gap and shows the feature of level repulsion, indicating a transition into a topologically trivial insulator phase, while the edge states in other plateau regions remain robust and gapless. This finding may explain the experimental observation of a divergent trend of the longitudinal resistivity at low temperatures near the Dirac points.

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