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From helical state to chiral state in ferromagnetic bilayer graphene



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ABSTRACT

We explore topological phases in biased ferromagnetic bilayer graphene, formed by bilayer graphene subjected to an external ferromagnetic exchange field, under a magnetic field. The most likely way to obtain a variety of distinct broken symmetry topological phases is proposed by means of ferromagnetic exchange field. Both spin-filtered quantum Hall and quantum spin Hall (QSH) phases are found. Edge modes in this QSH phase carry charge, spin and valley currents. When both time reversal and inversion symmetries are broken, the QSH phase remains robust against weak disorder. Moreover, topological phase transition from helical phase to chiral phase can be driven by simply tuning bias voltage or Fermi energy. A few possible experimental realizations are also discussed.

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1. Introduction

Graphene has generated a great interest since its discovery [1– 3]. The band structure of monolayer graphene is a Dirac-like spectrum in which conduction and valence bands with linear dispersion touch at the K and K' points in a Brillouin-zone corner [2]. The zero-energy anomaly due to the unique linear dispersion and particle-hole symmetry of Dirac cones gives rise to the halfinteger quantum Hall (QH) effect, characterized by chiral spindegenerate edge states [4,5]. In the presence of intrinsic spin-orbit coupling (SOC), graphene has been predicted to be a two-dimensional quantum spin Hall (QSH) system, characterized by helical edge states formed by counterpropagating edge states with opposite spins [6]. The bilayer graphene with the Bernal stacking is shown to have a quadratic band structure [7,8]. A tunable energy gap may open when a bias voltage is applied between the two layers [8-10], suggesting possible graphene-based tunable electronics and spintronics applications [11,12]. Due to its unusual band structure, the system shows a novel QH effect [7,13], unconventional QSH effect and quantum valley Hall (QVH) effect [14].

The QSH effect has attracted much attention since the pioneering works by Kane and Mele [6]. Now, it is well known that QSH effect is protected by time-reversal symmetry (TRS) and can be described by a Z_2 topological invariant. The intrinsic SOC in graphene opens a small non-trivial gap in the bulk and induces spin-filtered edge states inside the gap, which plays an important role in QSH effect. Nevertheless, the QSH effect is proved to be unobservable in pristine graphene [15,16], and was first experimentally observed in HgTe/CdTe quantum well [17].

Apart from the conventional QSH effect, two other kinds of TRSbroken QSH effects have been theoretically predicted in graphene so far. One is caused by intrinsic SOC combined with an exchange field [18] or a magnetic field [19–21]. Such QSH effect is unstable to spin-flip scattering due to magnetic disorder. However, recent progress shows that this QSH effect could become robust against general perturbations without any symmetry constrains [22]. The other is *CT*-invariant QSH effect in ferromagnetic graphene, involving a charge conjugation *C* and time reversal *T* operation [23].

In this work, we concentrate in topological phases in biased ferromagnetic bilayer graphene under a magnetic field. We consider the most promising way of achieving such topological phases by ferromagnetic exchange field. Depending on bias voltage or filling factor, and also on underlying magnetic field, a rich variety of electronic structures are realized. These interesting electron structures bring about plenty of topological phases, such as weak QSH, QSH, spin-filtered QH and spin-imbalanced QH phases. The tunability and electronic transport of topological phases are also addressed. In QSH phase, the edge states provide both spin and valley filtering, and therefore share the properties of both QSH and QVH phases. When time reversal and inversion symmetries are broken by magnetic field and bias voltage, the fate of the QSH phase is explored. Besides band structure engineering, bilayer

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Fig. 1. (Color on-line) (a) Low-energy spectrum of zigzag-edged bilayer graphene ribbon for the model without ferromagnetic exchange field for U = 0.05t and $\phi = 1/400$. The width of zigzag-edged ribbon is L=21.2 nm hereafter. The energy spectra for spin-up and spin-down components are completely degenerate. (b) The intervalley gap Δ_K in the $U-\phi$ plane. The color scale indicates the magnitude of the gap in units of *t*. The gap is zero in the white region.

graphene is an attractive candidate for transistor applications since it has a tunable gap. Hence, the theoretical feasibility of these results is proposed.

2. Model and method

The tight-binding Hamiltonian of ferromagnetic monolayer graphene which can be realized by depositing graphene on a ferromagnetic insulating substrate [24,25], under a perpendicular magnetic field B = (0, 0, -B) is [23]

$$H_{\rm MLG} = -t \sum_{\langle i,j\rangle,\alpha} e^{i\phi_{ij}} c^{\dagger}_{i,\alpha} c_{j,\alpha} - M \sum_{i\alpha} \alpha c^{\dagger}_{i,\alpha} c_{i,\alpha}, \qquad (1)$$

where $c_{i,\alpha}^{\dagger}$ and $c_{i,\alpha}$ are the electron creation and annihilation operators on site *i* with spin α , and *t* is the nearest neighbor hopping amplitude. The Peierls phase is denoted by $\phi_{ij} = \int_{r_j}^{r_i} A \cdot d\mathbf{r}/\phi_0$ with a integral over a line between sites *j* and *i*. The Landau gauge $\mathbf{A} = (0, -Bx, 0)$ is employed and $\phi_0 = \hbar/e$. In our calculations, the magnetic flux per hexagon is $\phi = 3\sqrt{3}/2a^2B/\phi_0$, where *a* is the lattice constant. *M* is the ferromagnetic exchange field.

The corresponding Hamiltonian of biased the Bernal-stacked ferromagnetic bilayer graphene takes the form [14]

$$H_{BLG} = H_{MLG}^{T} + H_{MLG}^{B} + t_{\perp} \sum_{\langle i,j \rangle, \alpha} (c_{i,\alpha,T}^{\dagger} c_{j,\alpha,B} + c_{j,\alpha,B}^{\dagger} c_{i,\alpha,T}) + U \sum_{i,\alpha} c_{i,\alpha,T}^{\dagger} c_{i,\alpha,T} - U \sum_{j,\alpha} c_{j,\alpha,B}^{\dagger} c_{j,\alpha,B},$$
(2)

where $H_{MLG}^{T,B}$ are the top (T) and bottom (B) layer Hamiltonians of Eq. (1), and $t_{\perp} = 0.13t$ is the nearest neighbors hopping of interlayer sites in the Bernal stacking. The bias voltage between two layers is 2*U* which can be controlled by chemical doping with nonmagnetic impurities or by adjusting the gate voltage [9,26].

To classify QSH phase, the spin Chern number [27] as well as Z_2 topological index is introduced and proved to yield equivalent descriptions for time-reversal invariant systems [27,28]. However, the spin Chern number unlike Z_2 invariance retains its robustness when TRS is broken. Therefore, we use the topological Chern number to discuss the topological property of the band structure. For graphene, the topological Chern number [29] and the spin Chern number [27,28] are defined as $C_c = C_+ + C_-$ and $C_s = (C_+ - C_-)/2$, where C_{\pm} is the Chern number for spin-up and spin-down sectors and can be expressed as $C_{\pm} = \sum_{\eta} C_{\pm}^{\eta}$ with η the valley index. The valley Chern number [30] per valley can be calculated from

$$C_{\alpha}^{\eta} = \frac{1}{2\pi} \sum_{n} \int_{BZ} dk_x \, dk_y \left(\Omega_{xy}^n \right)_{\alpha}^{\eta},\tag{3}$$

where $\alpha = \pm$ is the spin index and Ω_{xy}^n is the Berry curvature of the *n*th band given by

$$\Omega_{xy}^{n} = -2\sum_{n' \neq n} \frac{\operatorname{Im}\langle n | v_{x} | n' \rangle \langle n' | v_{y} | n \rangle}{(\varepsilon_{n} - \varepsilon_{n'})^{2}}.$$
(4)

The summation in momentum space is over all occupied bands below the bulk gap and $v_{x,y} = \partial H / \partial k_{x,y}$ is the velocity operator.

3. Results and discussion

Let us start by recalling the band structure of biased bilayer graphene under a perpendicular magnetic field. For biased bilayer graphene, the spatial inversion symmetry is broken and the valley degeneracy is lifted owing to the different natures of lowest Landau levels (LLs) in the two valleys. The resulting LLs are slightly split in each valley ($\eta = \pm$ for *K* and *K'*). For $n \ge 2$, the LLs are described by [13] $\varepsilon_n^{\pm} = \pm \hbar \omega_c \sqrt{n(n-1)} - \eta U$, where $\omega_c = eB/m$ is the cyclotron frequency, $m = t_{\perp}/2v_F^2$ is the effective mass of charge carriers, $v_F = (\sqrt{3}/2)at/\hbar$ is the Fermi velocity, and n = 0, 1, 2, ... is the LL index. Note that the accuracy of this expression is only correct in the limit $v_F \sqrt{2eB\hbar} \ll t_{\perp}$. For n = 0, 1, the low-energy LL spectrum is identified by $\varepsilon_0 = \eta U$ and $\varepsilon_1 = \eta U - \eta \delta$, where $\delta = U\hbar\omega_c/t_{\perp}$ is an induced splitting for every LL. There are also two specific LLs closest in energy to n=0,1 LLs, for simplicity, we label them by ηE_0 . The valley asymmetry has a stronger effect in the zero energy LLs and opens a bias-induced energy gap $\Delta_g = 2U$. The eightfold degenerate zero-energy LL (n=0 or 1) is split into four [9]. Two of which are forming two flat bands with energies U and -U, and the other two become dispersive inside the gap as shown in Fig. 1(a).

We numerically diagonalize the Hamiltonian in Eq. (2) to investigate the band structure of bilayer graphene. An intervalley gap Δ_K opens in a strong magnetic field [Fig. 1(a)]. To be more intuitive, we derive the topological phase diagram of the gap Δ_K as a function of both *U* and ϕ in Fig. 1(b). The intervalley gap does not emerge under weak magnetic field¹ $\phi_c \approx 1/640$ regardless of bias voltage [31]. At a fixed ϕ (> ϕ_c), the gap increases at first and then decreases to zero as bias voltage |*U*| increases. Here, we emphasize that the bias-driven intervalley gap, necessity for spin-filtered QH phase, can be obtained on both zigzag-edged and armchairedged bilayer graphene ribbons. However, for the armchair edge geometry, its valleys *K* and *K'* mix without a valley filter [14,32]. Thus, we only focus on zigzag edge geometry with open (periodic) boundary condition in the *x* (*y*) direction.

¹ This critical magnetic field is a numerical result with interlayer coupling $t_{\perp} = 0.13t$ and it will change with different interlayer couplings t_{\perp} .

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