Half-Quantized Hall Effect at the Parity-Invariant Fermi Surface

Jin-Yu Zou, Rui Chen, Bo Fu, Huan-Wen Wang, Zi-Ang Hu, and Shun-Qing Shen

Department of Physics, The University of Hong Kong, Pokfulam Road, Hong Kong, China

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Condensed matter realization of a single Dirac cone of fermions in two dimensions is a long-standing issue. Here we report the discovery of a single gapless Dirac cone of half-quantized Hall conductance in a magnetically-doped topological insulator heterostructure. It demonstrates that the Hall conductance is half-quantized in the unit $e^2/h$ when the parity symmetry is invariant near the Fermi surface. The gapless Dirac point is stable and protected by the local parity symmetry and the topologically nontrivial band structure of the topological insulator. The one-half Hall conductance observed in a recent experiment [Mogi et al, Nat. Phys. 18, 390 (2022)] is attributed to the existence of the gapless Dirac cone. The results suggest a condensed matter realization of a topological phase with a one-half topological invariant.

Introduction Search for a single gapless Dirac cone of fermions is a long standing issue in condensed matter physics [1–3]. In quantum field theory, an ideal massless two-dimensional Dirac fermion coupled to a U(1) gauge field gives rise to the parity anomaly, characterized by a half-quantized Hall conductance [4–8]. Lattice regularization of a single gapless Dirac cone on a lattice is not realizable if the parity symmetry is invariant according to the fermion doubling theorem [9]. One possible scheme is Wilson fermions which possess linear dispersion near the energy crossing point, but break the time reversal symmetry at higher energy [10, 11]. The proposal for the condensed matter realization of parity anomaly dates back to 1980s [12–14]. In his seminal paper [14], Haldane proposed that when one of the two valleys on a honeycomb lattice is finely tuned to be closed while another one remains open, a single flavor of massless Dirac fermion with parity anomaly can be realized. It is actually a critical transition point between a quantum anomalous Hall insulator and a conventional insulator. In graphene, the parity anomaly with half-integer quantum Hall effect is masked in view of the fourfold degeneracy from spin and valley in the system [15]. Due to the presence of the parity symmetry, the paired Dirac cones give rise to contributions to the anomaly terms with opposite signs thus exhibit no anomaly as a whole although the integer quantum Hall effect in graphene in a magnetic field has some clue of parity anomaly [16, 17]. A three-dimensional topological insulator hosts a single Dirac cone of fermions on its surface [18–21]. It provides a possible platform to observe the half-quantization of the Hall conductance, and a lot of attempts have been made in the direction [22–29]. Recently, the observation of the half-quantized Hall conductance in transport at zero magnetic field was reported as a signature of the parity anomaly in a semi-magnetic topological insulator heterostructure [30]. The paired gapless Dirac cones in a topological insulator thin film are located separately on the top and bottom surfaces. The local time reversal symmetry breaking on one surface by magnetic doping may open an energy gap for the Dirac surface fermions while the Dirac fermions remain gapless on the other surface. Existing theories suggest that the massive Dirac fermions give rise to half-quantized Hall conductance [22, 23]. However, it is known that all the independent bands on a two-dimensional finite Brillouin zone just have an integer Chern number [31, 32]. The gapless Wilson fermions in two-dimensions have a half-quantized Hall conductance when the valence bands are fully filled [33, 34]. Thus the semi-magnetic topological insulator becomes a potential candidate to realize a single gapless Dirac cone in condensed matter. In this Letter, we report the discovery of the gapless Dirac cone of half-quantized Hall conductance in a semi-magnetic topological insulator heterostructure.
main results are summarized in Fig.1. The gapless Dirac cone always has one half quantized Hall conductance in the units of $e^2/h$ when the parity symmetry is invariant near the Fermi surface. The gapless Dirac point is protected by the local parity symmetry and the topologically nontrivial band structure of the topological insulator, although the parity symmetry was broken at higher energy. The gapped Dirac cone has a nonzero Hall conductance, but becomes zero when the band is fully filled. So the massive Dirac fermions alone do not contribute a half-quantized Hall conductance.

The exchange interaction between the magnetic ion and the magnetic element Cr was doped on the top surface. Numerical calculation shows a condensed matter realization of the topological phase with a one-half topological invariant.

**Band structure of a semi-magnetic topological insulator** A semi-magnetic topological insulator film consists of topological insulator (Bi, Sb)$_2$Te$_3$ and Cr-doped (Bi, Sb)$_2$Te$_3$ grown by molecular-beam epitaxy. (Bi, Sb)$_2$Te$_3$ is a topological insulator with an energy gap of about 0.3eV, and hosts a single Dirac cone of the surface electrons [35–37]. As shown in Fig. 1(e), the magnetic element Cr was doped on the top surface. The exchange interaction between the magnetic ion and the surface electrons leads to nonzero magnetization and opens an energy gap on the top surface electrons [38–41]. The Fermi energy can be finely tuned by changing the ratio of Bi and Sb such that it locates within the band gap of the top surface Dirac cone. The material has been extensively studied since the discovery of topological insulator, although the topological nature of (Bi, Sb)$_2$Te$_3$ can be well described by a tight-binding model for the electrons of $P_{2\uparrow}$ and $P_{2\downarrow}$ orbitals from (Bi, Sb) and Te atoms near the Fermi energy [25, 35, 42].

$$H_{TI} = \sum_i \Psi_i^\dagger M \Psi_i + \sum_{i, \alpha=x,y,z} \left( \Psi_i^\dagger \Gamma_\alpha \Psi_{i+\alpha} + \Psi_{i+\alpha}^\dagger \Gamma_{\alpha} \Psi_i \right)$$

(a)

where $M = (m_0 - 2 \sum \alpha t_\alpha) \sigma_0 \tau_z$, $\Gamma_\alpha = t_\alpha \sigma_0 \tau_z - i \frac{\lambda_\alpha}{2} \sigma_\alpha \tau_x$, $\Psi_i^\dagger$ and $\Psi_i$ are the four-component creation and annihilation operators at position $i$. The Pauli matrices $\sigma_\alpha$ and $\tau_\alpha$ act on the spin and orbital indices, respectively. All bands are doubly degenerate due to the coexistence of both time-reversal and inversion symmetries in the absence of magnetic doping. It can produce the linear dispersion of the surface states near the Fermi point in an open boundary condition. The exchange interaction caused by Cr doping is given by a $V_{exch} = \sum_i \Psi_i^\dagger V(i) \sigma_z t_0 \Psi_i$, which is only present on the lattice sites of the top layers with the magnitude as $V_z$. In experiments, the thickness of the Cr-doped (Bi, Sb)$_2$Te$_3$ is about 2nm and (Bi, Sb)$_2$Te$_3$ layer is about 8nm [30]. We take the periodic boundary condition in the $x$- and $y$-direction and open boundary condition in the $z$ direction, the calculated dispersions are presented in Fig. 2a. It is noted that there exist a gapless Dirac cone and a gapped Dirac cone within the bulk gap. The dispersions for the gapless Dirac cone cross at the Fermi point and are linear in $k$ around the crossing point. The gapped Dirac cone opens an energy gap of about $2V_z$, which is caused by the exchange interaction of Cr-doping on the top surface. Numerical calculation shows that the gapless and gapped states within the bulk band gap are mainly located on the bottom and top surfaces, respectively. We check the energy separation between the two bands along the high symmetric lines, and find that the gapless Dirac cone and gapped Dirac cone are well separated. The dip at $k_z$ indicates that there exists a band mixture. Finite thickness of the film may cause a tiny gap at the Fermi point, which decays exponentially in the thickness approximately [43, 44]. With increasing exchange interaction, the gap is quickly suppressed by several order of magnitudes to negligibly small (about $10^{-16}$E, for a thickness $L_z = 10$nm, see Fig. 2c). It will be smeared out easily by temperature broadening (1K is about 0.086meV) in experimental measurements.

The Hall conductance and the Berry curvature Using the Kubo formula for the electric conductivity [45], we calculate the Hall conductance as a function of the chemical potential $\mu_F$ numerically for the tight-binding model in Eq. (1) with a thickness $L_z = 10$nm. A fairly flat plateau of $-e^2/4\pi$ appears within the band gap as shown in Fig. 3a. To figure out the origin of the conductance...
plateau, we first note that there exists a full band gap between four lowest energy bands and the rest at all $k$. These four bands form well-separated band-subspaces and the Hall conductance as a function of $\mu_F$ can be calculated for each band. We then only focus on the gapless and gapped Dirac cones denoted by red and violet lines in Fig. 2a. For the gapped Dirac cone, we have a nonzero Hall conductance as $\mu_F$ varies, which has its maximal about $0.4\frac{e^2}{h}$, but decays to zero quickly when the band is fully occupied. The maximal value may increase for a thicker film, but always be lower than $0.5\frac{e^2}{h}$. This is consistent with the fact that the Chern number of a well-defined band in a finite Brillouin zone is always an integer (including zero) \[ \frac{21}{32} \]. For the gapless Dirac cone, the Hall conductance becomes $-0.5\frac{e^2}{h}$ within the bulk band gap, which is larger than the gap of the gapped Dirac cone. Thus the total Hall conductance within the bulk band gap are mainly contributed by these two bands and the Hall conductance plateau is attributed to the gapless Dirac cone instead of the gapped Dirac cone. 

To explore the topological nature of the gapless Dirac cone and its relation to the Hall conductance, we studied the Berry curvature of the gapless bands. In the Bloch states $|u_{n,k}\rangle$, the Berry connection and the Berry curvature are defined as $A_{n,o}(k) = i\langle u_{n,k}|\partial_k u_{n,k}\rangle$ and $\Omega_2^n(k) = \partial_k A_{n,o}(k) - \partial_o A_{n,k}(k)$, respectively \[ \frac{21}{32} \]. For the gapless Dirac cone, it is found that the Berry curvature $\Omega_2^n(k) = 0$ within the regime of $k < k_c$. Beyond the regime, it becomes negative and finally vanishes for a larger $k$. Combining with the band structure, the nonzero Berry curvature mainly originates from hybridization of the states from the top and bottom layers. The conductance plateau appears when the chemical potential is located in the regime where the Berry curvature vanishes. 

On the parity-invariant regime. Now we come to discuss the origin of the parity-invariant regime based on the tight-binding model in Eq. (1). For each wave vector $k$, the Hamiltonian can be divided into two parts, $H_{T}(k) = H_{1d}(k) + H_{S}(k)$. $H_{1d}$ is equivalent to a one-dimensional lattice model with a gap $m_0(k) = m_0 - 4t_{\parallel\parallel} \left( \sin^2 \frac{k_x a}{2} + \sin^2 \frac{k_y a}{2} \right)$ \[ \frac{21}{32} \],

$$H_{1d}(k) = \sum_{i_z} \left( \Psi_{i_z,k}^{\dagger} M(k) \Psi_{i_z,k} + \Psi_{i_z,k}^{\dagger} T \Psi_{i_z+1,k} + h.c. \right)$$

with $M(k) = \begin{bmatrix} m_0(k) - 2t_{1z} \end{bmatrix} \sigma_0 \tau_z$, and $H_{S}(k) = \lambda \sum_{i_z=a=x,y} \Psi_{i_z,k}^{\dagger} \sin(k_z a) \sigma_0 \tau_x \Psi_{i_z,k}$. For $m_0(k) > 0$, i.e. $k < k_c \simeq \sqrt{M/t_{1z}/a}$, $H_{1d}$ is topologically nontrivial. There exist a pair of zero energy modes at each side or near the top surface and bottom surface. Denote $\xi_s$ and $\chi_t$ the two eigenvectors of $\sigma_x$ and $\tau_y$ with eigen values $s = \pm 1$ and $t = \pm 1$. The zero energy modes are the eigen vectors $\xi_s \otimes \chi_t$ of the operator $\sigma_x \tau_y$ with the eigenvalue $S = st$. The spatial part of the two states of $S = 1$ ($s = 1, t = 1$) and $S = -1$ are mainly located near the top surface and the two states of $S = -1$ are located near the top surface, and decay exponentially to its opposite side \[ \frac{21}{32} \]. By mapping $H_S(k) + V_{exch}$ into the the basis of the four states, one obtains the effective Hamiltonian the gapless Dirac cone $H_b(k) = -\lambda_t (\sin(k_z a) \sigma_y - \sin(k_y a) \sigma_x)$ which is mainly located at the bottom layer and the gapped Dirac cone $H_b(k) = +\lambda_t (\sin(k_x a) \sigma_y - \sin(k_y a) \sigma_x) + V(k) \sigma_z$ which is at the top layer. $V(k)$ is given by the expectation of the exchange interaction $V_{exch}$, and varies with the wave vector, especially when $m_0(k) \rightarrow 0$ where the wave function of zero energy modes evolve to distribute broadly in space. In two dimensions, the parity symmetry is defined by $P H(k) P^{-1} = H(Mk)$, where $P = i\sigma_y$ and $M$ is the mirror operator in momentum space transforming $k \rightarrow Mk = (k_x, -k_y)$. Thus in the regime the gapless Dirac cone $PH_b(k)P^{-1} = H_b(Mk)$ respects the parity symmetry while the gapped Dirac cone $PH_b(k)P^{-1} \neq H_b(Mk)$ breaks the symmetry due to the presence of $V(k)$. Thus the nontrivial condition of $m_0(k) > 0$ defines a parity-invariant regime for the gapless Dirac cone. In additional to the local parity symmetry, $H_b$ also respects a space-time operator $I_{ST} = C_{2z} T$ where $C_{2z}$ is a twofold rotation about the $z$ axis, and $T$ is local time reversal operator. $I_{ST} = +1$ imposes a further constraint on the Berry curvature, leading to $\Omega_2^n(k) = 0$. When $m_0(k) < 0$, $H_{1d}$ becomes topologically trivial. The zero energy modes evolve into the bulk states with nonzero energy.. The states are no longer the
eigen-vectors of the operator $\sigma_z \tau_y$, and break the parity symmetry. Based on this picture, we propose an effective four-band model

$$H_F = \lambda_{||} (\sin k_x a \sigma_y - \sin k_y a \sigma_x) \gamma_z + V(k) \sigma_z (\gamma_z + 1) + H_{\Delta}^{\text{eff}}$$

(3)

where $H_{\Delta}^{\text{eff}} = f(k) m_0(k) \gamma_x$ describes the hybridization of the states. A Fermi-Dirac-distribution-like factor or the sigmoid function $f(k) = \frac{1}{1 + \exp \left( \frac{m_0(k)}{\Delta} \right) + 1}$ is introduced to describe the procedure that the coupling is eventually turned on at higher energy. $\gamma_{x,z}$ are the Pauli matrices representing the top and bottom layers. A small $T^*$ is a model-specific parameter. The calculated results show that the model can reproduce the key features of the band structure. The Hall conductance as a function of $\mu_F$ is given by $\sigma_H^n = \frac{e^2}{h} (S - \cos \phi_S (k_F^S))$. The part of $S$ is mainly attributed to the hybridization term $H_{\Delta}^{\text{eff}}$ and the band splitting $V(k)$. For the gapless band of $S = -1$, $\cos \phi_S (k_F) = 0$ in the parity-invariant regime and $\sigma_{\Delta}^1 = \frac{-e^2}{8 \pi}$. For the gapped band of $S = +1$, $\cos \phi_S = 1$ for the full occupancy and $\sigma_{\Delta}^1 = 0$. They are in a good agreement with the numerical results in Fig. 3b. The details are referred to Ref. [47].

Half-quantization and parity symmetry Now we present a relation between the half-quantization of the Hall conductance and the parity symmetry. In the Hal-dane model and the Wilson fermions, it was found that the Hall conductance is half-quantized when the chemical potential is located at the energy crossing point $\mu_F = \frac{\epsilon_0}{2 \pi}$ [14]. Here we prove that the Hall conductance is one half of an integer if the parity symmetry is respected near the Fermi level $\mu_F$. In two dimensions, the intrinsic Hall conductance for band $n$ can be expressed in terms of the Berry gauge field in momentum space [92],

$$\sigma_H^n (\mu_F) = \frac{e^2}{h} \int \frac{d^2 k}{2 \pi} C \partial \phi \cdot A_{\sigma} \phi (\varepsilon_{\sigma} n, k - \mu_F)$$

(4)

where $\theta(x)$ is the step function, i.e., $\theta(x) = 1$ for $x < 0$ and zero otherwise. The whole Brillouin zone can be divided into two patches by the Fermi level $\mu_F$, the occupied and unoccupied regime, respectively. By using the Stokes’ theorem, the integral of the Berry curvature over the occupied regime can be converted into the integrals over the Fermi surface (FS), $\sigma_H^n (\mu_F) = \frac{-e^2}{4 \pi h} \oint_{FS} d \vec{l} \cdot \nabla \phi \cdot A_{\sigma} \phi$. Here $\vec{l}$ is the wave vector along the Fermi surface. Consider the case that the Hamiltonian $H(k)$ is invariant under the parity symmetry along the Fermi surface, i.e. $\mathcal{P} H(k) \mathcal{P}^{-1} = H(\bar{k})$. The eigenstates of $H(k)$ at $k$ and $\bar{k}$ on the Fermi edge must be related by a gauge transformation: $\mathcal{P} |u_n(k) \rangle = \exp (i \theta_0(k)) |u_n(\bar{k}) \rangle$. Accordingly, the Berry connection is transformed to $A_{\sigma} \phi (\varepsilon_{\sigma} n, k) = \partial \phi \cdot \theta_0(k) + \sum B_{\alpha \beta} \partial \phi \cdot \theta_0(k)$. The determinant of the Jacobian matrix $J_{ab}$ equals $-1$. It follows that $2 \sigma_H^n = \frac{e^2}{h} \oint_{FS} d \vec{l} \cdot \nabla \phi \cdot \theta_0(k) = \frac{e^2}{h} \nu$. For a linear dispersion near the Dirac point, the Berry phase around the Fermi surface is $+\pi$ or $-\pi$, depending on the helicity of the Dirac fermions. Correspondingly $\nu$ is equal to +1 or −1. Thus the Hall conductance $\sigma_H = \frac{\nu e^2}{4 \pi h}$ is half quantized in the case that the parity symmetry is restored near the Fermi level.

Disorders and robustness of the quantized Hall conductance The robustness of the half-quantized Hall conductance comes from two aspects. One is the local parity invariance for the gapless Dirac cone. The exchange interaction is only present at the top surface. The low-energy dispersion of the gapless Dirac cone is mainly located at the bottom layer, and is less affected by the exchange interaction, although the part of higher energy is modified. The other aspect is that the presence of the surface states is mainly attributed to the three-dimensional band structure of the topological insulator. It is known that the topology of the band structure of three-dimensional topological insulator is very robust against the disorders. If the strength of disorders is not strong enough to induce a topological phase transition, the gapless surface states are still present. In this way the Dirac point is very stable against the disorders before the phase transition occurs.

To illustrate the robustness of the single Dirac cone in this quasi-two-dimensional system, we calculated the Hall conductance as a function of the strength of disorders. We follow the common practice in the study of Anderson localization to introduce disorder through random non-magnetic on-site energy with a uniform distribution with $[-W/2, +W/2]$. We calculate the Hall conductance of a disordered square of size $L_x \times L_y \times L_z$ for a fixed thickness $L_z$ by means of the noncommutative Kubo formula [49],

$$\sigma_H = i 2 \pi \text{Tr} \{ \mathbf{P} \left[ -i [x, \mathbf{P}], -i [y, \mathbf{P}] \right] \} \frac{e^2}{h}$$

(5)

with the periodic boundary conditions along the $x$ and $y$ directions. Here, $x$ and $y$ are the coordinate operators and $\text{Tr} \{ \cdots \}$ is the trace over the occupied bands. $\mathbf{P}$ is the projector onto the occupied states of the system. Figure 4 shows the numerically calculated disorder-averaged Hall conductances as functions of the disorder strength. In the clean limit, the system exhibits the half-quantized Hall conductance as expected. With increasing disorder strength, the Hall conductance remains about $0.5 \frac{e^2}{h}$ until the disorder strength $W$ exceeds about 0.83eV. The critical disorder strength is much larger than the exchange interaction and also larger than the bulk energy gap of topological insulator. Further increasing the disorder strength, the conductance drops quickly and the system is expected to be localized by disorders. Thus, the half-quantized Hall conductance is robust against the disorder. This demonstrates explicitly that the gapless Dirac cone is quite stable against the disorders.

The presence of impurities will cause the scattering between electron wave functions which leads to an energy level repulsion effect [50]. The stability of the Dirac point
is thus equivalent to examine the relative energy level repulsion between the two states at Dirac point from all other surface and bulk states. The scatterings between two bottom surface states will not introduce Dirac mass renormalization due to the presence of the local time-reversal symmetry, and the accompanying Fermi level $\mu_F = 0.01$ eV and the lattice spacing $a = 1$ nm. 200 random configurations are adopted to average for each value.

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Figure 4. The Hall conductance as a function of the strength of nonmagnetic disorders $U/\sigma_0 T_0$ for several lattice sizes $L_x \times L_y \times L_z$ for a fixed $L_z = 10$ nm. The Fermi level $\mu_F = 0.01$ eV and the lattice spacing $a = 1$ nm. 200 random configurations are adopted to average for each value.
