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Effects of spin-flip scattering on gapped Dirac fermions

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Abstract – We investigate the effects of spin-flip scattering on the Hall transport and the spectral properties of gapped Dirac fermions. We find that in the weak scattering regime, the Berry curvature distribution is dramatically compressed in the electronic energy spectrum, becoming singular at band edges. As a result, the Hall conductivity has a sudden jump (or drop) of $e^2/(2h)$ when the Fermi energy sweeps across the band edges, and otherwise is a constant quantized in units of $e^2/(2h)$. The spectral properties such as the density of states and the spin polarization are also greatly enhanced near band edges. Possible experimental methods to detect these effects are discussed.

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Introduction. – The Dirac fermion has found its ubiquitous appearance in interesting physical systems such as graphene [1] and topological insulators [2,3]. The most important feature of the Dirac fermion is its strong (pseudo)spin-orbit coupling, which is directly encoded in the Hamiltonian and underlies many unusual effects. When a certain symmetry breaking mechanism is introduced, a gap can be opened up at the Dirac point. The gapped Dirac fermion (GDF) is in some sense more interesting in that its electronic band develops a Berry curvature gauge field [4,5] which acts like a magnetic field in the momentum space, and deflects electron flow in transverse directions leading to the anomalous Hall effect [6].

Disorder scattering usually has strong effects on the Hall transport even in the weak disorder limit when the system is in a metallic state. So far, most studies of scattering effects on Dirac fermions have focused on spin-independent scattering. However, due to the strong spin-orbit coupling, it is natural to expect that the carrier motion should have a sensitive dependence on the change of spin state during a scattering.

In this paper, we study the effects of spin-flip scattering on the properties of GDFs. Our work is motivated by recent advances in creating GDF on the surface of topological insulators [7,8] and the ability of systematic control of surface carrier density through doping or gating [9]. We

show that in the weak scattering regime spin-flip scattering compresses the Berry curvature distribution dramatically towards the band edge. Hence, whenever the Fermi energy is tuned across a band edge, the Hall conductivity has a sudden change of $e^2/(2h)$, *i.e.* half of the conductance quantum. Away from the band edges, the Hall conductivity is a constant independent of the carrier density. Since the Hall transport is central to several exotic physical effects [10] proposed recently for topological insulators, the discovery presented here is expected to have important observable consequences. We also find that spectral properties like the density of states (DOS) and spin polarization, which are usually not very sensitive to disorder scattering, get greatly enhanced near band edges by the spin-flip scattering, which can be detected by photoemission spectroscopy or tunneling spectroscopy measurements.

Quantized Hall conductivity and Berry curvature compression. – A GDF is described by the Hamiltonian

$$\hat{\mathcal{H}}_0 = v_F \mathbf{k} \cdot \boldsymbol{\tau} + \Delta \tau_z, \quad (1)$$

where v_F is the Fermi velocity, $\mathbf{k} = (k_x, k_y, 0)$, and $\boldsymbol{\tau} = (\tau_x, \tau_y, \tau_z)$ is a vector of Pauli matrices acting on the spin degrees of freedom. Without the second term, the Hamiltonian is for a massless Dirac fermion with a cone-like energy dispersion. The term $\Delta \tau_z$ induces a finite mass and opens up an energy gap of 2Δ in the spectrum. Such a term can be generated by breaking the time-reversal

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symmetry at the surface of a topological insulator, for example, through magnetic doping [7] or coating with insulating ferromagnetic films.

Because of the strong spin-orbit coupling and the spin splitting induced by the mass term, an anomalous Hall effect in the absence of external magnetic field is expected. In the weak scattering regime, the anomalous Hall conductivity has an important contribution σ_{xy}^0 from the momentum space Berry curvature of the spin-orbit coupled bands [6]. It is known as the intrinsic contribution because it is an intrinsic property of a crystal. For a two-dimensional (2D) system the intrinsic contribution is given by the integral of momentum space Berry curvature $\Omega_{n\mathbf{k}}$ of all the occupied states $|n\mathbf{k}\rangle$ (n is the band index), $\sigma_{xy}^0 = -\frac{e^2}{h} \frac{1}{A} \sum_{n\mathbf{k}} \Omega_{n\mathbf{k}} f_{n\mathbf{k}}$, where A is the area of the 2D system, $f_{n\mathbf{k}}$ is the Fermi distribution function,

$$\Omega_{n\mathbf{k}} = - \sum_{n' \neq n} \frac{2 \text{Im} \langle n\mathbf{k} | v_x | n'\mathbf{k} \rangle \langle n'\mathbf{k} | v_y | n\mathbf{k} \rangle}{(\omega_{n'\mathbf{k}} - \omega_{n\mathbf{k}})^2}, \quad (2)$$

v_i ($= v_F \tau_i / \hbar$ with $i = x, y$ for GDF) is the velocity operator and $\hbar \omega_{n\mathbf{k}}$ is the energy of the state $|n\mathbf{k}\rangle$. The distribution of Berry curvature in the energy spectrum can be described by the density of Berry curvature $\Omega(\varepsilon) \equiv \frac{1}{A} \sum_{n\mathbf{k}} \Omega_{n\mathbf{k}} \delta(\varepsilon - \hbar \omega_{n\mathbf{k}})$. Then the intrinsic contribution can be put into the form $\sigma_{xy}^0 = -\frac{e^2}{h} \int d\varepsilon \Omega(\varepsilon) f(\varepsilon)$.

For GDFs, the density of Berry curvature and the intrinsic contribution of Hall conductivity can be easily calculated using the formulae above. The result is

$$\Omega(\varepsilon) = -\frac{\Delta}{4\pi\varepsilon^2} \text{sgn}(\varepsilon) \Theta(|\varepsilon| - |\Delta|), \quad (3)$$

$$\sigma_{xy}^0(\varepsilon_F) = -\frac{e^2}{2h} \left[\frac{\Delta}{|\varepsilon_F|} \Theta(|\varepsilon_F| - |\Delta|) + \text{sgn}(\Delta) \Theta(|\Delta| - |\varepsilon_F|) \right], \quad (4)$$

where $\Theta(x)$ is the Heaviside step function and ε_F is the Fermi energy. As shown by the blue curves in fig. 1, while the density of Berry curvature has its maximum (or minimum) value at band edges, its distribution spreads over the whole energy spectrum, hence the value of σ_{xy}^0 changes gradually as a function of the Fermi energy. For each band the total weight of Berry curvature corresponds to a contribution of $\pm e^2/(2h)$ to the Hall conductivity, where the sign difference reflects the different helicities of the two bands. It needs to be mentioned that the half-quantized contribution from the filled lower band does not contradict the well-known fact that the contribution from a completely filled band must be integer quantized [6]. This is because the Dirac model is energetically unbounded. It can only serve as a low-energy effective model for any real physical systems, where the evaluation of the contribution from all the completely filled bands obviously has to go beyond the effective model. On the other hand, it is crucial to notice that the disorder-related contribution, which is our focus in this paper, is tied to the Fermi surface hence is well captured within such effective model.

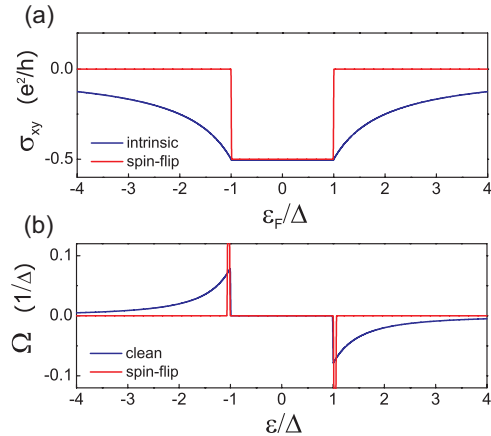


Fig. 1: (Color online) (a) The anomalous Hall conductivity and (b) the density of Berry curvature for the gapped Dirac fermion (with $\Delta > 0$) as a function of energy. The blue curve in (a) is for the intrinsic contribution and the red curve is for a disordered system with weak spin-flip scattering. The Berry curvature is compressed by the scattering to be singular at band edges, as shown schematically in (b).

The existence of disorder scattering is essential for stabilizing the electron distribution under a drive field and establishing the dynamic steady state. In the case of the anomalous Hall effect, the role of disorder scattering is especially important yet complicated. In the weak scattering regime, when expanded in terms of the disorder density n_{dis} , the leading contribution to σ_{xy} is generally of order n_{dis}^{-1} , known as the skew scattering contribution which originates from the asymmetry in the scattering rate and depends on the details of the disorder model [6]. The next leading order (of n_{dis}^0 dependence) consists of the intrinsic contribution discussed above and the side jump contribution [6]. The skew scattering contribution and the side jump contribution arise from disorder scattering, they are referred to as extrinsic contributions. The side jump contribution is peculiar in that it arises from scattering but is independent of both the scattering strength and the disorder density. Due to its presence, even for disorder models with vanishing skew scattering (such as Gaussian disorder models), the Hall conductivity σ_{xy} in the weak disorder limit $n_{\text{dis}} \rightarrow 0^+$ does not correspond to the value of the intrinsic contribution σ_{xy}^0 [6]. This is an important point that needs to be emphasized.

In a recent study of the anomalous Hall effect [11], we find that the extrinsic contributions to σ_{xy} depend sensitively on the spin structure of disorder scattering. This is understandable because the Hall transport is a result of spin-orbit coupling, different actions on the spin state during a scattering will also strongly affect the carrier's orbital motion. Here we are most interested in the effects of spin-flip scattering on the gapped Dirac fermions. Such kind of scattering can be modeled as a random potential $U(\mathbf{r}) = \sum_{\alpha} \mathbf{B}^{\alpha}(\mathbf{r} - \mathbf{R}_{\alpha}) \cdot \boldsymbol{\tau} = B_x(\mathbf{r})\tau_x + B_y(\mathbf{r})\tau_y$, with \mathbf{B}^{α} being a random in-plane vector. We assume that

the random field satisfies the correlation $\langle B_i(\mathbf{q})B_j^*(\mathbf{q}') \rangle_c = n_{\text{dis}}u^2\delta_{ij}\delta(\mathbf{q}-\mathbf{q}')$, where $i, j \in \{x, y\}$, $B_i(\mathbf{q})$ is the Fourier component of $B_i(\mathbf{r})$, $\langle \cdots \rangle_c$ stands for disorder average and u is the scattering strength. We assume that the system has no preferred in-plane direction, such that the random vector \mathbf{B}^a is uniformly distributed in plane. Then the third-order disorder correlation $\langle UUU \rangle_c$ must vanish identically. Because the skew scattering contribution depends on the third-order correlation [6,12], this means that the skew scattering process is forbidden for this kind of disorder. Therefore, the leading-order contribution to the Hall conductivity comes from the intrinsic and the side jump terms which are independent of scattering strength and disorder density.

In the weak scattering regime, the Hall conductivity can be evaluated perturbatively using the Kubo-Streda formula [13]. The calculation has been detailed in our previous work [11]. Here we quote the final result which is that the side jump contribution is

$$\sigma_{xy}^{\text{sj}}(\varepsilon_F) = \frac{e^2}{2\hbar} \frac{\Delta}{|\varepsilon_F|} \Theta(|\varepsilon_F| - |\Delta|), \quad (5)$$

hence the total Hall conductivity is given by

$$\sigma_{xy}(\varepsilon_F) \simeq \sigma_{xy}^0 + \sigma_{xy}^{\text{sj}} = -\frac{e^2}{2\hbar} \text{sgn}(\Delta) \Theta(|\Delta| - |\varepsilon_F|). \quad (6)$$

This is a very interesting result. As plotted in fig. 1(a), σ_{xy} has a sudden jump or drop of half the conductance quantum at the band edges. As soon as the Fermi energy passes the band edge, the value of σ_{xy} becomes a constant quantized in units of $e^2/2\hbar$. The effect of the spin-flip scattering makes the anomalous Hall conductivity quantized in the whole energy spectrum, which is different from other types of disorders [11,12].

In this paper, we would like to promote another perspective on the unusual phenomena described by eq. (6). Instead of starting from a clean system and treating disorders as perturbations, we start directly from a disordered system and try to generalize the concept of Berry curvature for the disordered case. For each eigenstate $|\alpha\rangle$ with eigenenergy $\hbar\omega_\alpha$ of the disordered system, we define its Berry curvature as

$$\Omega_\alpha \equiv -\sum_{\beta \neq \alpha} \frac{2 \text{Im} \langle \alpha | v_x | \beta \rangle \langle \beta | v_y | \alpha \rangle}{(\omega_\beta - \omega_\alpha)^2}. \quad (7)$$

We further introduce a Berry curvature operator $\hat{\Omega} \equiv \sum_\alpha \Omega_\alpha |\alpha\rangle \langle \alpha|$, such that the density of Berry curvature can be generalized as

$$\Omega(\varepsilon) \equiv \frac{1}{A} \text{Tr} \left[\hat{\Omega} \delta(\varepsilon - \hat{\mathcal{H}}) \right]. \quad (8)$$

It follows from the Kubo formula that the Hall conductivity for disordered systems can be expressed as

$$\sigma_{xy} = -\frac{e^2}{\hbar} \int d\varepsilon \langle \Omega(\varepsilon) \rangle_c f(\varepsilon), \quad (9)$$

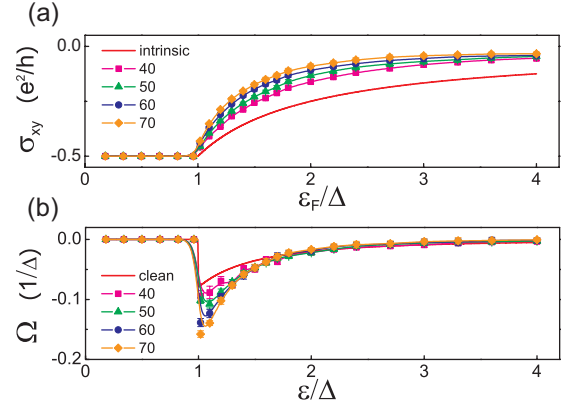


Fig. 2: (Color online) Numerical result of (a) the Hall conductivity and (b) the Berry curvature distribution for increasing system sizes with $N_k = 40, 50, 60, 70$ averaged over 200, 100, 80, 50 samples, respectively. In the calculation we set $v_F = \Delta = 1$, the momentum cutoff $K_c = 6$, and the strength $|B_i(\mathbf{q})|$ ($i = x, y$) is a random number uniformly distributed in an interval $[0, W]$ with $W = 0.03$ (accordingly, $n_{\text{dis}}u^2 \simeq W^2 K_c^2/3 \sim 0.01$). The error bar stands for one standard deviation.

with a disorder averaged density of Berry curvature. This is an exact result. We again emphasize that although the definition of generalized Berry curvature recovers that for a perfect crystal when the eigenstates $|\alpha\rangle$ are simply Bloch states $|n\mathbf{k}\rangle$, the weak disorder limit ($n_{\text{dis}} \rightarrow 0^+$) of eq. (9) is not equal to the intrinsic contribution. It also contains the side jump contribution (for vanishing skew scattering). Mathematically, this is because the disorder-averaged Berry curvature contains nontrivial vertex corrections which do not vanish in the weak disorder limit. From eq. (6) we find that in the weak disorder limit

$$\langle \Omega(\varepsilon) \rangle_c = -\frac{1}{4\pi} \text{sgn}(\varepsilon\Delta) \delta(|\varepsilon| - |\Delta|). \quad (10)$$

As shown schematically in fig. 1(b), the density of Berry curvature, which is originally spread over the energy spectrum, gets compressed dramatically towards the band edges by the scattering, while its total weight ($\pm \frac{1}{4\pi}$ for the lower and the upper band, respectively) is kept unchanged.

Based on eqs. (7)–(9) we perform a numerical calculation to further confirm our analytic result. Due to the particle-hole symmetry, σ_{xy} is a symmetric function with respect to $\varepsilon_F = 0$, hence here we only focus on the positive energy range. The calculation is performed in momentum space on disordered systems of size $N_k \times N_k$. Figure 2 shows the results for σ_{xy} and Ω with different system size N_k . The physically meaningful value of a transport coefficient such as σ_{xy} corresponds to the thermodynamic limit when $N_k \rightarrow \infty$. The result in fig. 2 indeed shows that the density of Berry curvature is squeezed by the weak spin-flip scattering to the upper-band bottom. Consequently the contribution to the Hall conductivity from the upper band approaches a half-quantized plateau in the energy spectrum, which confirms our analytic result.

To completely understand the microscopic mechanism of this peculiar disorder effect is difficult. Nevertheless, we notice that for the gapped Dirac fermion, the spin-flip scattering has weak scattering rates near the band bottom because states there have large spin z -components, while large scattering rates occur for high energies where the spins are more or less lying in the plane. Our result indicates that the Berry curvature tends to be expelled from the strong scattering region towards the weak scattering region while keeping its total weight unchanged, hence making the curvature distribution squeezed towards band bottom. This is similar to the migration of the Chern number carrying states driven by impurity scattering observed in the quantum Hall effect [14,15].

Enhanced DOS and spin polarization. – Spectral properties such as the DOS are usually considered to be insensitive to weak disorder scattering. This is particularly true when the DOS does not vary much in the energy range under consideration, such as for a 2D free-electron gas where the DOS is a constant. A GDF gas without disorder has a DOS

$$\rho_0(\varepsilon) = \frac{|\varepsilon|}{2\pi v_F^2} \Theta(|\varepsilon| - |\Delta|). \quad (11)$$

There are three salient features of this DOS that are crucial for the effects to be discussed below: 1) ρ_0 increases linearly from the band edge; 2) ρ_0 has a finite value $\frac{|\Delta|}{2\pi v_F^2}$ at band edges; 3) ρ_0 does not depend on the value of the spin splitting Δ as long as $|\varepsilon| > |\Delta|$. Figure 3(a) shows the numerical result of the DOS for a clean system together with the DOS for a disordered system with spin-flip disorders. It is observed that spin-flip scattering strongly enhances the DOS near the band edge, and slightly decreases the DOS at large energies, as being required by the conservation of the total number of states.

This effect can be qualitatively understood from the self-energy correction due to scattering. In the Born approximation, (assuming $\varepsilon > \Delta > 0$ in the following), the 2×2 retarded self-energy is given by $\Sigma^R = \frac{1}{A} \sum_{\mathbf{k}} \langle U G_0^R(\mathbf{k}, \varepsilon) U \rangle_c$, with

$$\text{Re } \Sigma^R(\varepsilon) = -\frac{n_{\text{dis}} u^2}{2\pi v_F^2} \ln \left| \frac{\varepsilon^2 - \varepsilon_c^2}{\varepsilon^2 - \Delta^2} \right| (\varepsilon \tau_0 - \Delta \tau_z), \quad (12)$$

and $\text{Im } \Sigma^R(\varepsilon) = -\frac{n_{\text{dis}} u^2}{2\pi v_F^2} (\varepsilon \tau_0 - \Delta \tau_z)$, where ε_c is the energy cutoff and τ_0 is the 2×2 identity matrix. While the imaginary part of the self-energy only contributes to a small level broadening in the weak scattering regime, the real part has a large magnitude near the band edge and diverges logarithmically as $\varepsilon \rightarrow \Delta$. In fact, this disorder-induced singularity is a generic feature for systems having a finite (unperturbed) DOS at the band edge, as is the case for the GDF system.

Thermodynamic properties can be extracted from the Green function $G^R = (\varepsilon - \mathcal{H}_0 - \Sigma^R)^{-1}$. From eq. (12), the self-energy only corrects the energy argument ε and spin

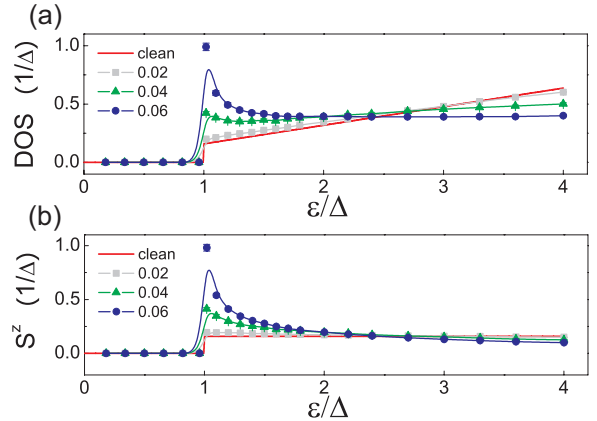


Fig. 3: (Color online) Numerical results of (a) the DOS and (b) the spin polarization S^z for increasing disorder strength with $W = 0.02, 0.04, 0.06$ with each data point averaged over 50 samples, where W is defined in the caption of fig. 2. In the calculation, we set $N_k = 70$, and $v_F = \Delta = 1$.

splitting Δ in G^R . It follows that the disordered DOS can be approximated as

$$\rho(\varepsilon) \simeq \rho_0[\varepsilon(1 + \lambda), \Delta(1 + \lambda)], \quad (13)$$

with the right-hand side standing for the DOS at energy $\varepsilon(1 + \lambda)$ for a clean GDF system with Δ replaced by $\Delta(1 + \lambda)$, where $\lambda = \frac{n_{\text{dis}} u^2}{2\pi v_F^2} \ln \left| \frac{\varepsilon^2 - \varepsilon_c^2}{\varepsilon^2 - \Delta^2} \right|$ is the prefactor appearing in eq. (12). Near the band edge, λ is a positive number, hence $\rho(\varepsilon) \simeq (1 + \lambda)\rho_0(\varepsilon)$ is enhanced by a factor of $(1 + \lambda)$ compared with the clean case¹. Now it is clear that a strong enhancement of DOS by scattering requires the original DOS has a large variation on the energy scale of $\lambda\Delta$. Therefore, such effect does not occur for a conventional 2D free-electron gas, and although the GDF near the band edge resembles the 2D free-electron gas, the self-energy correction makes the Dirac behavior at higher energies relevant. Similarly, the spin polarization $S^z(\varepsilon) = -\frac{1}{\pi A} \text{Im Tr}[\tau_z G^R(\varepsilon)]$ is also enhanced at the band edge by the factor $(1 + \lambda)$, as shown in fig. 3(b).

Discussion. – The exotic effects reported here arise from the interplay between the GDF and the spin-flip scattering. There are two important properties of GDFs underlying these effects: the Berry curvature and the unusual DOS. Disorder scattering modifies these fundamental properties in the spectrum, thereby strongly influences the system behavior.

Spin-conserving scattering such as $B_0(\mathbf{r})\tau_0$ or $B_z(\mathbf{r})\tau_z$ also affects the anomalous Hall transport of the GDF

¹A more careful evaluation leads to the result that $\rho(\varepsilon) = \rho_0(\varepsilon) \left[1 + \frac{n_{\text{dis}} u^2}{2\pi v_F^2} \left(\ln \left| \frac{\varepsilon^2 - \varepsilon_c^2}{\varepsilon^2 - \Delta^2} \right| - 2 \right) \right]$, which shows that the curves of $\rho(\varepsilon)$ and $\rho_0(\varepsilon)$ have a crossing point at the energy ε_* when $\ln \left| \frac{\varepsilon_*^2 - \varepsilon_c^2}{\varepsilon_*^2 - \Delta^2} \right| - 2 = 0$. With the parameter values in our numerical calculation, we find that $\varepsilon_* = 2.55$ which agrees very well with the result in fig. 3(a).

system in metallic state. In contrast with the spin-flip scattering, their skew scattering contribution is in general nonvanishing. Their side jump contributions are also distinct from that of the spin-flip scattering [11,12]. In particular, the Berry curvature is not compressed into a small region in the spectrum. The combined effects of different kinds of scattering would depend on the competition between them [11,16]. As for the disorder-modified DOS, the spin-conserving scattering has a similar effect as the spin-flip scattering. This can be understood by noticing that the self-energy correction for spin-conserving scattering only differs from eq. (12) by a sign change of Δ . Because ρ_0 does not depend on Δ (for energies within the bands), the result is similar to that for the spin-flip scattering. Meanwhile, the spin polarization becomes $S^z(\epsilon) \simeq (1 - \lambda)S_0^z(\epsilon)$. In the energy range where $\lambda > 1$, the spin polarization can even have a sign change.

GDF has been realized on the surface of topological insulators [7]. This is partly motivated by the possibility to achieve a half-quantized anomalous Hall effect by tuning the Fermi level into the surface band gap [3,17]. In contrast, our focus here is instead on the energy range outside the gap. We notice that for a purely 2D system with embedded gapped Dirac spectrum, it is possible to realize a half-quantized anomalous Hall effect in the metallic state with the help of spin-flip scattering. For example, consider a Hamiltonian $\mathcal{H}_0 = v_F(\sin k_x \tau_x + \sin k_y \tau_y) + (\Delta + 2 - \cos k_x - \cos k_y)\tau_z$ ($\Delta > 0$) which corresponds to a tight-binding lattice model proposed to model the Mn-doped HgTe/CdTe quantum wells [18]. It has a direct gap at the Γ -point of the Brillouin zone. The low-energy effective model near the gap is just that for a GDF. As we mentioned before, the contribution to the Hall conductivity from the completely filled lower band (or any remote valence band) must be integer quantized. Therefore, once the Fermi energy is slightly above the upper-band bottom and spin-flip scattering is turned on, an $e^2/(2h)$ contribution arises from the upper-band bottom making the total Hall conductivity half-quantized. In fact, the noninteger value of Hall conductivity dictates that the system must be conducting [19]. The effect itself would be very interesting since it realizes a fractional quantized Hall effect for noninteracting electrons in a metallic state, plus it does *not* require the completely filled valence bands to have a nontrivial topology, *i.e.* with a nonzero Chern number [5].

Finally, we briefly comment on the possible experimental methods to detect the effects studied here on the surface of topological insulators. The surface band gap can be opened by depositing an ultrathin insulating ferromagnetic film on top of a topological insulator such that a proximity-induced exchange coupling can be introduced. Spin-flip scattering can be realized by thermally excited spin waves in the ferromagnetic film. However, to make spin wave scattering dominate over other scattering processes is a nontrivial task. It requires a temperature range where spin wave excitation dominates over phonon excitation and improved sample quality such that

very few impurities are present near the interface. Ferromagnetic insulating materials such as EuS and EuO with the Curie temperature much lower than the Debye temperature are possible candidates. The Hall conductivity can be measured through standard multi-terminal setup. The sudden change of Hall conductivity at band edges will also manifest itself in the signal of magneto-electric or magneto-optic effects [10]. Enhanced DOS and spin polarization at band edges can be directly detected through the photoemission spectroscopy or the tunneling spectroscopy measurements, which should be much easier.

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