1. Introduction

A topological insulator is a new quantum state of matter [1–3], in which a couple of helical or chiral conducting boundary states reside in the bulk insulating gap stably. Novel quantum spin Hall effect (QSHE) [4–7] and quantum anomalous Hall effect (QAHE) [8–12] have been suggested in topological insulator systems. Comparing to the QSHE, QAHE is more promising in future device applications since it is robust against magnetic disorder scattering. QAHE was originally discussed in various two-dimensional models with broken time-reversal symmetry, especially the honeycomb lattice [8] and monolayer/bilayer graphene systems [9, 10]. Recently, QAHE was theoretically proposed in magnetic topological insulators (MTIs) [13, 14]. Soon after, the existence of QAHE in three-dimensional (3D) magnetically doped (Bi,Sb)$_2$Te$_3$ films was confirmed by a series of experiments [15–18].

In a 3D TI, the conducting surface holds massless Dirac Fermions. In the presence of ferromagnetic exchange field along $z$-direction, the time-reversal symmetry is broken and the nontrivial gap is opened in the top and bottom gapless surfaces with opposite-signed effective mass shown in figure 1(a),...
which induces non-dissipative chiral edge states and consequently the ideal QAHE with perfectly quantized Hall resistance $h/e^2$ and zero longitudinal resistance. However, in the experimental observations [15–17], the chiral edge states of QAHE are usually dissipative, where the Hall resistance $\rho_{xy}$ is quantized but the longitudinal resistance $\rho_{xx}$ significantly deviates from zero. The origin of this derivation attracts intensive research interests and various mechanisms has been suggested, for instance, thermally activated carriers [17], the alignment of exchange fields [18], the existence of extra non-chiral edge states, [19, 20] etc. All these delicate interpretations are based on ideal 2D models. However, an MTI thin film is a quasi-2D system in $x$-$y$ plane but has finite thickness in $z$-direction. Different from [8, 9] and [21, 22], in which QAHE is considered in ideal 2D systems or superposition of ideal 2D systems, QAHE in MTI thin films is contributed by two half-integer quantum Hall conductances from the top and bottom Dirac-like surfaces with opposite-signed effective mass [23, 24]. The edge states of QAHE actually propagate through side surfaces of MTI films. Therefore, the geometric structure of the side surface along $z$-direction, as a result of nano-fabrication, is important in the formation of QAHE in MTI thin films.

In this work, we study the effect of geometric mismatch on QAHE in MTIs. As shown in figure 1(b), due to the geometric mismatch, the chiral edge state of QAHE is backscattered near the entrance of the central Hall bridge (the red arrowed lines), as though it is scattered by defects (gray ellipse) in the Hall bridge. This additional scattering is similar to the effect of splitting gates in the Hall effect, in which part of edge states is backscattered due to the pinchoff of the Hall bridge depicted in figure 1(c) [25]. Using the effective 3D tight-binding Hamiltonian and the non-equilibrium Green’s function (NEGF) method, we numerically calculate the longitudinal resistance $\rho_{xx}$ and Hall resistance $\rho_{xy}$ of this six-terminal system. Assuming the probability of the additional scattering in Hall bar is $p$, the longitudinal resistance and Hall resistance are found to be $\rho_{xx} \approx p(h/e^2)$ and $\rho_{xy} = h/e^2$, respectively. This result provides reasonable explanations on the deviation from ideal QAHE in recent experiments [15–18]. It is also found that additional scattering due to the non-ideal contact can be suppressed and finally eliminated by strong magnetic fields, which is in agreement with experimental observations. Meanwhile, Anderson-type disorders induced by magnetic doping can also suppress the dissipation of $\rho_{xx}$.

The paper is organized as follows. In section 2, we present theoretical analysis on the dissipative edge states of QAHE in MTIs. In section 3, we numerically calculate $\rho_{xx}$ and $\rho_{xy}$ of a 3D MTI system using NEGF method, through which we present how the theoretical analysis is related to the experimental observation. Finally, a summary of our work is presented in section 4.

2. Theoretical analysis

In an MTI film, the helical surface states are gaped in the top and bottom surfaces and gapless in the side surfaces, as shown in figure 1(a). When the Fermi energy is located in the
surface energy gap induced by the exchange field $M_z$, the surface states are localized. Therefore, only the chiral zero mode [26] propagates along the surface boundaries (the red arrows in figure 1(a)). In this case, the chiral states (the gray arrows in figures 1(b)–(f)) should dominate the transport in the six-terminal Hall system, leading to the $\nu = 1$ QAH state. For the multi-terminal nonequilibrium transport system, the macroscopic electrodes are usually macroscopic. Because of the macroscopic electrode, although electrons keep flowing into or out of leads, the Fermi distribution of each lead remain unchanged in the multi-terminal nonequilibrium system. The macroscopic electrodes are usually contacted or attached with the micro sample through leads. The width or thickness of leads is usually comparable with the central region. In the experimental setup, the metallic electrodes are pinned on the MTI film, which could induce mismatch between electrodes and the central MTI sample. Due to the finite thickness in the $z$ direction, the contact between the Hall bar and the external leads could be incomplete or broken to some extent. As a result, the edge states are scattered at the entrances of the Hall bar or the entrances of external leads, which leads to the backscattering edge states or floating edge states, as shown in the figures 1(b) and (d)–(f), respectively. In the following, we analyze these two situations in detail.

(1) The floating edge states. In this case, electrons are influenced by the boundaries of the external leads (the thick black lines in figures 1(d)–(f)). As a result, additional scattering for floating edge states occurs near the entrances of six terminals as shown in figures 1(d)–(f). In figures 1(d) and (e), terminal 2 ‘sees’ only the channels originating from terminal 3, so $V_2 = V_3$. In figure 1(f), terminal 3 ‘sees’ only the channels coming from terminal 4 and $V_3 = V_4$, and terminal 2 ‘sees’ the channels originating from both terminal 3 and terminal 4. Since $V_3 = V_4$, we have $V_2 = V_3 = V_4$. It means that there is no voltage drop along the longitudinal direction. In another word, the longitudinal resistance $\rho_{xx} \approx 0$ in the presence of floating edge states.

Besides the intuitive analysis, we can also derive the expressions of $\rho_{xx}$ and $\rho_{xy}$ from the Landauer-Büttiker formula [25]. The current flowing from terminal $m$ to the central scattering region can be calculated as

$$J_m = \frac{e^2}{h} \sum_n T_{mn}(V_m - V_n) \quad (1)$$

where $m, n = 1, 2, \ldots, 6$. $V_m$ is the voltage on terminal $m$, and $T_{mn}$ is the transmission coefficient from terminal $n$ to terminal $m$. In equation (1), we have used the gauge invariance condition $\sum_n T_{mn} = \sum_n T_{nm}$. In the measurement of QAHE, a bias $V$ is applied across terminal 1 and terminal 4 to inject current, as shown in figure 1. The other terminals 2, 3, 5 and 6 are voltage probes and have zero currents, i.e. $J_2 = J_3 = J_5 = J_6 = 0$. Using the boundary conditions $V_1 = V$, $V_4 = 0$, $J_2 = J_3 = J_5 = J_6 = 0$, together with the transmission matrix $T_{mn}$, we can calculate the currents $J_1 = -J_4$ and the voltages $V_2$, $V_3$, $V_5$ and $V_6$ by solving equation (1). Then, the longitudinal resistance $\rho_{xx} \equiv (V_2 - V_1)/J_1$ and Hall resistance $\rho_{xy} \equiv (V_6 - V_5)/J_1$ are obtained.

Assuming $p$ is the probability of the additional scattering shown in figures 1(d)–(f), the transmission matrix elements of the Hall device can be written as $T_{n,n-2} = p$ (if $n = 1$ or 2, $n - 2 = 5$ or 6), $T_{n,n-1} = 1 - p$ (if $n = 3$, and others are zero. Taking into account the boundary conditions, the Landauer-Büttiker formula can be written as $\mathcal{J} = \mathcal{T} \mathcal{V}$ with $\mathcal{J} = (J, 0, 0, -J, 0, 0)^T$, $\mathcal{V} = (1, V_2, V_3, 0, V_5, V_6)^T$, and

$$\mathcal{T} = \begin{pmatrix}
1 & p - 1 & p & 0 & 0 & 0 \\
0 & 1 & p - 1 & p & 0 & 0 \\
0 & 0 & 1 & p - 1 & p & 0 \\
0 & 0 & 0 & 1 & p - 1 & p \\
1 & 0 & 0 & 0 & 1 & p - 1 \\
p - 1 & p & 0 & 0 & 0 & 1
\end{pmatrix} \quad (2)
$$

Solving the above linear equations $\mathcal{J} = \mathcal{T} \mathcal{V}$, we get the injecting current and the boundary voltages

$$J = \frac{e^2}{h} \frac{1}{1 + p - p^2}, \quad V_2 = \frac{p(1 - p)}{1 + p - p^2}, \quad V_3 = \frac{p}{1 + p - p^2}, \quad V_5 = \frac{1}{1 + p - p^2}, \quad V_6 = \frac{1 - p^2}{1 + p - p^2} \quad (3)$$

From equation (3), the longitudinal resistance and Hall resistance are expressed as

$$\rho_{xx} = -\frac{\hbar}{e^2} \frac{p^2}{1 - p^3} \approx -\frac{p^2}{e^2}, \quad \rho_{xy} = \frac{1}{e^2} \frac{1 - p}{1 - p^3} \approx (1 - p) \frac{\hbar}{e^2} \quad (4)$$

These results suggest that, in the presence of floating edge states, $\rho_{xx}$ is almost zero for small $p$ and $\rho_{xy}$ is driven away from the quantized value, which is different from the experimental observation.

(2) The backscattering edge states. In this case, electrons in the central region are impacted by the boundary of the Hall bar (the thick black lines in figure 1(b)). Similar to the previous case, additional scattering also occurs near the entrance of the Hall bar, as shown in figure 1(b). The situation is equivalent to the case of splitting gates [25] shown in figure 1(c), in which terminal 3 (6) ‘sees’ only the channels originating from terminal 4 (1). Hence,

$$V_3 = V_4, \quad V_6 = V_1 \quad (5)$$

Assuming the probability of additional scattering is $p$, i.e. $T_{26} = T_{35} = p$. Since terminal 2 (5) ‘sees’ channels originating from both terminal 3 (6) and terminal 6 (3) with weights of $1 - p$ and $p$, respectively, we
get $V_2 = (1 - p)V_4 + pV_6$, $V_5 = (1 - p)V_4 + pV_3$. Comibined with the conditions in equation (5), we have

$$V_2 = (1 - p)V_4 + pV_1, \quad V_5 = (1 - p)V_4 + pV_4.$$  \hspace{1cm} (6)

Finally, we can obtain the longitudinal bias $V_2 - V_3 = p(V_1 - V_4)$, which means $\rho_{xx} \propto p$. In addition, the net current of terminal 1 is determined by the incoming current (to the central scattering region) and the outgoing current (from the central scattering region) in the form of $J_1 = J_{1,\text{in}} - J_{1,\text{out}}$. According to figure 1(b), $T_{26} = T_{53} = p$, $T_{23} = T_{56} = 1 - p$ and other $T_{mn} = 1$, one easily gets

$$J_{1,\text{in}} = \frac{\hbar}{e^2} \sum_n T_{n1} V_1 = T_{12} V_1,$$

$$J_{1,\text{out}} = \frac{\hbar}{e^2} \sum_n T_{1n} V_n = T_{12} V_2,$$

$$J = J_1 = \frac{e^2}{\hbar} (V_1 - V_2) = \frac{e^2}{\hbar} (1 - p)(V_1 - V_4).$$  \hspace{1cm} (7)

Then, from equation (5)–(7), we can derive $\rho_{xx}$ and $\rho_{xy}$ as

$$\rho_{xx} = \frac{\hbar}{e^2} \frac{p}{1 - p} \approx p \frac{h}{e^2}, \quad \rho_{xy} = \frac{\hbar}{e^2}.$$  \hspace{1cm} (8)

Obviously, in the presence of the backscattering, $\rho_{xy}$ is perfectly quantized and $\rho_{xx}$ is slightly dissipative. This conclusion provides a reasonable explanation to the origination of nonzero $\rho_{xx}$ and quantized $\rho_{xy}$ of QAH effect in a series of experiments performed on MTIs.

From these theoretical analysis, we have shown that the additional scattering at the entrances of the Hall bar leads to the backscattering edge states. It is these backscattering edge states that induces the dissipative edge states for QAH in an MTI film. In the following numerical calculation, we will numerically study how the geometric mismatch between the detecting leads and the central region impacts the QAH effect of MTI films, and find the relation between the geometric mismatch and backscattering.

3. Numerical results and discussions

In this section, we present quantitative results of geometric effect on QAH. In order to study the geometric effect on the system’s thickness described by $z$, instead of the 2D TI system [27, 28], we construct a six-terminal scattering device fabricated on the magnetically doped (Bi, Sb)$_2$Te$_3$ film with finite thickness. In the following, we numerically calculate the longitudinal resistance $\rho_{xx}$ and the Hall resistance $\rho_{xy}$ with a 3D tight-binding Hamiltonian and non-equilibrium Green’s function formalism.

We first introduce the Hamiltonian of an MTI film fabricated on (Bi, Sb)$_2$Te$_3$. Starting from the $k \cdot p$ model, the Hamiltonian of magnetically doped (Bi, Sb)$_2$Te$_3$ is expressed as [29, 30]

$$H_0 = A_{\perp} k_z \sigma_z \tau_z + A_{\parallel}(k_x \sigma_x + k_y \sigma_y) \tau_x$$

$$+ M_1 \sigma_0 \tau_z + M_2 \sigma_ \tau_0 + \epsilon_k$$  \hspace{1cm} (9)

where $\sigma_0$ and $\tau_0$ are $2 \times 2$ unitary matrices, $\sigma_{xy}$ and $\tau_{xy}$ are Pauli matrices, representing the real spin and and pseudo spins. The Hamiltonian (9) is write in the basis of four low-lying states $|P_1^+, \uparrow (\downarrow) \rangle$ and $|P_2^+, \uparrow (\downarrow) \rangle$ at the $\Gamma$ point. $A_{\perp}$, $A_{\parallel}$ and $M_1$ depict the coupling between low-lying states. $\epsilon_k$ is the on-site energy, $\epsilon_k$ and $M_2$ are momentum dependent with $M_2 = D_0 - D_1 k_z^2 - D_2 (k_x^2 + k_y^2)$ and $\epsilon_k = C_0 + C_1 k_x^2 + C_2(k_z^2 + k_y^2)$. ‘$\perp$’ and ‘$\parallel$’ represent the direction perpendicular to the $x$-$y$ plane or parallel with the $x$-$y$ plane, respectively. $M_1$ is the exchange field induced by the magnetic dopants along the $z$-direction. Considering $\epsilon_k$ can only change the energy band globally, and has no impact on the topological properties, we set $\epsilon_k = 0$ for an intuitive analysis. The other parameters are $A_{\perp} = 2.2 \ eV \ Å$, $A_{\parallel} = 4.1 \ eV \ Å$, $D_0 = -0.28 \ eV$, $D_1 = -10 \ eV \ Å^2$, $D_2 = -56.6 \ eV \ Å^2$, respectively [30]. Using the finite-difference approximation, we can get the effective nearest tight-binding Hamiltonian of the 3D MTI system in square lattice [33]

$$H = \sum_i d_i^\dagger H_i d_i + \sum_{(ij)} d_i^\dagger H_{ij} d_j$$  \hspace{1cm} (10)

with

$$H_i = \epsilon_i \sigma_0 \tau_0 + (D_0 - 2 \sum_{\alpha} \frac{D_\alpha}{a^2} \sigma_0 \tau_0 + M_2 \sigma_\tau_0$$

$$H_{ij} = \delta_{\mathbf{k}l} A_{\alpha i + a_{\alpha j}} \left[ \frac{D_\alpha}{a^2} \sigma_0 \tau_0 - \frac{A_{\alpha i}}{2a} \sigma_\tau_0 \tau_x \right] e^{i\phi_{l} d_{i} + a_{\alpha j}}$$

where, $d_i = [d_i^{(1)}, d_i^{(2), \perp}, d_i^{(4), \parallel}, d_i^{(4), \perp}, d_i^{(4), \parallel}, d_i^{(4), \perp}, d_i^{(4), \parallel}, d_i^{(4), \perp}]$. $H_i$ and $H_{ij}$ depicts the Hamiltonian at the same site and the coupling between the nearest sites, respectively. $\alpha = x, y, z, F_x = F_y = F_z = F_\parallel$. $F_\parallel = A, D$, $\epsilon_i$ is the on-site energy induced by the random disorders, $a = |a|$ is the lattice constant of the cubic lattice. Equation (10) is based on the finite difference method. The lattice constant $a$ is approximately the distance between two adjacent lattice sites. The calculation will converge as long as the lattice constant is small enough. Here, we set $a = 5 \ Å$.

Further, as in the experiments, an external magnetic field is applied to eliminate the residual bulk conducting states [31, 32]. Hence the vector potential induced by the magnetic field is also considered in our calculation, which are related as $B = \nabla \times A$. To guarantee the gauge invariance, the nearest coupling satisfies $\langle \psi_x | \psi_y \rangle = e^{i(\theta(x,y) - \theta(x,y))} | \psi_x | \psi_y \rangle$, where $\langle \psi_x | \psi_y \rangle$ and $\langle \psi_y | \psi_x \rangle$ are the coupling between nearest sites with and without magnetic field $B = [0, 0, B]$, respectively. Accordingly, an extra phase $e^{i \phi_{l} d_{i} + a_{\alpha j}} = e^{i \theta(x,y) d_{i} + a_{\alpha j}} A \cdot d_i$ is induced in the nearest neighbor coupling term $H_{ij}$. For the six-terminal devices shown in figure 1, lead-1, lead-4 are infinite in $x$-direction. Then, in the Coulomb gauge, the vector potential is chosen as $x$-independent $A = [-B y, 0, 0]$ in lead-1, lead-4 and the central scattering region. For lead-2, lead-3, lead-5 and lead-6 which are infinite in $y$-direction, $A = [0, B x, 0]$ is used. For each layer in the $x$-$y$ plane, the magnetic flux through each unit cell satisfies $\Phi_0 = BA^2$. At the boundaries between the scattering region and lead-2, lead-3, lead-5 and lead-6, constant magnetic field is maintained through the gauge transformation.
By tuning the relative composition of Bi and Sb, the Fermi surface can be shifted into the bulk gap. In the numerical calculation, we set $E_F = 0.01\text{eV}$ which is within the energy gap. Other computational parameters include: the exchange field $M_z = 0.15\text{eV}$; the widths of the scattering region $L_y = 30a$ which is the same as the width of six leads; the length of the central scattering region $L_z = 90a$. The thickness of leads $L_x$ and the thickness of the central region $L_{cz}$ vary in the calculation. From equation (1) the transmission matrix elements between the six terminals are calculated through non-equilibrium Green’s functions are needed. It is expressed as

$$T_{mn} = \text{Tr}[\Gamma_m G \Gamma_n G'^\dagger].$$

Here ‘Tr’ denotes the trace over real space and orbital space $|P2\rangle/|P1\rangle$. The linewidth function is $\Gamma_m = i[\Sigma_m - \Sigma_m'^{-1}]$ and the retarded Green’s function is defined as $G' = G'^{-1} = (E - H_c - \sum_m \Sigma_m)^{-1}$ where $H_c$ is the Hamiltonian of the central scattering region and $\Sigma_m = H_{cm}K_mH_{mc}$ is the retarded self-energy function contributed by the $m$th terminal lead. $g_m'$ is the surface Green’s function of the $m$th lead, which can be calculated iteratively through transfer matrix [34, 35] or Bloch eigenvector [36, 37]. Finally, we can get the longitudinal resistance $\rho_{xx}$ and Hall resistance $\rho_{xy}$ from the Landauer-Büttiker formula in equation (1).

To show the impact of the film thickness, in figure 2 we display the thickness-dependent band structures of an infinite MTI slab. Here, we set typical $L_y, L_{cz} = 6a$ and $12a$ for thin films, which is around 1 and 2 quintuple layers in experiment. When the exchange field $M_z = 0$, the bulk states of a wide film should be gapless. The finite-size gap in figure 2(a1) will vanish if $L_y$ is large enough, as shown in the tendency of figures 2(a1) and (a3). Comparing figures 2(a1) and (a2), we can find the film thickness $L_y$ of the slab impacts the bulk energy bands but does not affect the topological properties of the system. As long as $M_z = 0$, no topological edge states appear in the band structures. In the presence of an exchange field $M_z = 0.15\text{eV}$, the energy bands of top and bottom surfaces (along the $x$-$y$ plane) are gaped and topological edge states emerge in figure 2(b). The topological edge states can only propagate through the gapless edge states. In this case, the existence of edge states is independent of the film thickness $L_z$, but the magnitude of the bulk band gap is determined by $L_z$, as shown in the difference between figures 2(b1) and (b2). The slab width $L_x$ merely impacts the bulk energy bands, and does not affect the width of the band gap, as shown in figures 2(b1) and (b3), which is different from the case of $M_z = 0$. Therefore, the geometry in $z$ direction is vital for QAHE in MTI films.

Then, in order to study how the geometric structure in the third dimension $z$ affects the QAHE in MTI films, we explore a series of six-terminal devices with different $L_{xz}$ and $L_{yz}$, which is shown in the top sketches of figure 3. In these sketches, from the left to the right, the geometric structure of the devices evolves gradually from the slim structure ($L_{xz} = L_{yz} = 3a$), to the convex structure ($L_{xz} < L_{yz}$), the thick structure ($L_{xz} = L_{yz} = 30a$), the concave structure ($L_{xz} > L_{yz}$), and finally back to the slim structure ($L_{xz} = L_{yz} = 3a$). For the convex structure with $L_{xz} = 3a$ and $L_{yz} = 30a$ (the second sketch of top panels of figure 3), the transmission coefficients are $T_{2y} = T_{3y} = 0.04$, $T_{1z} = T_{5z} = 0.002$. Comparing to $T_{26}$, the transmission $T_{62}$ from lead-2 to lead-6 can be neglected.
This coincides with the scattering mechanism depicted in figure 1(b). Further, corresponding to the device sketches in the top panels, \( L_{cz} \) and \( L_{lz} \) are plotted in figures 3((a1) and (a4)) and ((b1)–(b4)), respectively. It is found that for the convex geometry (the left panels of figure 3), the longitudinal resistance \( \rho_{xx} \) increases promptly from zero, reaches to the maximum when \( L_{cz} \) is the largest and then decreases back to zero rapidly with the increase of \( L_{lz} \) as shown in figures 3(a1) and (a2). At the same time, the Hall resistance \( \rho_{xy} \) increases slowly from \( \hbar e^2 / 2h \) and basically maintains quantized as shown in figures 3(b1) and (b2). Comparing to the ideal QAHE, \( \delta \rho_{xx} \), which is consistent with the experimental observations [15]. Therefore, we conclude that the convex structure can give rise to additional backscattering near the entrance of the terminals may induce a negative \( \rho_{xx} \), which agrees with equation (4). The concave geometry induces larger deviation of \( \rho_{xy} \) than \( \rho_{xx} \), which is inconsistent with the experiments. Considering the broken leads, the concave geometry is unreasonable in experiment. Therefore, we predict that the geometric mismatch, such as the convex structure, can induce the deviation of \( \rho_{xy} \) while maintaining the perfectly quantized \( \rho_{xx} \).

However, the convex structure is not straightforward in the experimental setup. In experiment, the macroscopic electrodes are pinned on the MTI film. To a considerable extent, the effective contact between the electrodes and the film is incomplete or even poor, which induces backscattering edge states. In order to simulate more realistic situations, we elaborate more delicate geometric structures. In figure 4, we plot \( \rho_{xx} \) and \( \rho_{xy} \) versus external magnetic field \( B \) for three different contact patterns as shown in the top panels of figure 4. When the leads and the central region are perfectly contacted, i.e. \( L_{cz} = L_{lz} = 3a \), all of the lattice sites in the lead (the black dots) are contacted to the central region (the up-left sketch). Then, the ideal QAHE is observed with \( \rho_{xx} = 0 \) and \( \rho_{xy} = \hbar / e^2 \). The perfect QAHE is kept for a broad range of magnetic fields (the black dotted lines in figures 4(a1) and (a2)). Then the extreme case, i.e. convex structure with \( L_{lz} = 10a \) and \( L_{cz} = 30a \) (the up-middle sketch in figure 4), is evaluated, in which the thickness of the leads (the black dots) is much smaller than that of the central region (including the grey dots). As shown in figure 1(b), additional backscattering near the entrance of the Hall bar induces larger nonzero \( \rho_{xx} \) and the nearly quantized \( \rho_{xy} \) (the red solid lines in figures 4(a1) and (a2)). In addition, in this poor contact situation, \( \rho_{xx} \) and \( \rho_{xy} \) oscillates with the variation...
of the magnetic field strength. The oscillation period satisfies \( \Delta B(L_x L_y) \approx h/e \), which means the magnetic flux through the central sample is approximately the magnetic flux quantum.

In a more general situation, the lattice sites of the lead (the black dots) through which the central region is connected to the external electrodes, are randomly distributed, as shown in the up-right sketch in figure 4(b). We define the contact ratio \( r \) between coupled lattices and total lattices. For a very poor contact \( r = 0.2 \), both \( \rho_{xx} \) and \( \rho_{xy} \) deviate from ideal values to the same extent (the black dotted lines in figures 4(b1) and (b2)). With the increasing of \( r \), \( \rho_{xy} \) approaches to the quantized value \( h/e^2 \) gradually, while \( \rho_{xx} \) is roughly kept in the same order as in the case of \( r = 0.2 \). This fact shows that the geometric structure has a remarkable impact on \( \rho_{xx} \), but almost does not affect \( \rho_{xy} \).

Next, we study the effect of the magnetic field. As demonstrated in experiments [15–18], the Hall resistance \( \rho_{xy} \) is quantized while the longitudinal resistance \( \rho_{xx} \) is nonzero in zero or weak magnetic fields, i.e. the edge states are slightly dispersive. The only way to eliminate this dissipation is applying an external magnetic field. In some case, a strong magnetic field (\( |B| > 5T \)) can finally eliminate the dissipation. [15] However, if the incomplete contact is significant, \( \rho_{xx} \) does not go to zero even in a very strong magnetic field of 10T [16]. It shows that the geometric effect is also vital in QAHE of MTI films.

From figure 4(b), we can find that \( \rho_{xy} \) is nonzero at \( B = 0 \). At relatively good contact (\( r = 0.4 \) and 0.9), with the increasing of \( B \), \( \rho_{xx} \) is quickly depressed to zero, while \( \rho_{xy} \) just slightly oscillates. Our results confirm the experimental observation that \( \rho_{xx} \) is much more sensitive to the magnetic field than \( \rho_{xy} \). For a moderate contact with \( r = 0.4 \) (blue curve in figure 4(b1)), \( \rho_{xx} \) quickly drops to zero as the magnetic field is increased, which is in good agreement with the observation of [15]. In contrast, for a good contact (\( r = 0.9 \), red curve in figure 4(b1)) the dissipative component \( \rho_{xx} \) is smaller but it goes to zero at a slower rate in the presence of magnetic field, as in [16]. In addition, our numerical data show that \( \rho_{xx} \) has small oscillations as a function of the magnetic field which was also observed in experiments [16]. It should be noted that, the chirality of the edge states in the QAH system and the quantum Hall system is opposite in the presence of a negative magnetic field. Therefore,
when the magnetic field is reversed from positive to negative (−3T < B < 0 region in figure 4(b)), a trivial band cross will lead to the singularities of ρxx and ρxy. The same phenomena have also been observed in experiments [15, 16].

Finally, the disorder effect is evaluated, since magnetic doping on MTIs can induce static disorders. The Anderson-type static disorder is modeled through the random on-site energy, which uniformly distributes in the interval [−w/2, w/2] with w the disorder strength. Here, we consider the perfect contact situation, i.e. Lcz = Llz = 10a. Numerical results show that in this case the Hall resistance ρxy is hardly affected by the Anderson-type disorder. Therefore, in figure 5, we plot only the longitudinal resistance ρxx and its fluctuation Δρxx versus the disorder strength w for different magnetic fields B. It is found that, moderate disorder can induce the localization of residual bulk states and suppress the longitudinal resistance so that ρxx ≈ 0 and Δρxx ≈ 0, while the edge states remain intact. In this process, the fluctuation of ρxx is slightly peaked (left part of figure 5(b)). Near w = 1.8 eV, an ideal QAHE occurs with zero fluctuation of ρxx. This is very similar to topological Anderson insulators in quantum spin Hall effect [38, 39]. When the disorder is further increased, the backscattering between the chiral edge states located on the opposite edges will destroy the QAHE states. As a result, ρxx and Δρxx abruptly increases. Our numerical results show that, the chiral edge states are immune to weak disorder. Moreover, appropriate disorder is beneficial for the QAHE by suppressing the dissipative edge states, which provides useful insight on future experiments.

4. Summary

In summary, we expound the dissipative edge states of QAHE in MTIs with simple and intuitive physics. We have shown by both theoretical analysis and numerical evidence that, due to the geometric mismatch between the leads and the central sample, the backscattering edge states are induced and give rise to the nonzero longitudinal resistance ρxx and quantized Hall resistance ρxy. In more general cases, the incomplete contact between leads and the central region contributes to the backscattering edge states. It is numerically found that, the nonzero ρxx can be effectively suppressed by external magnetic fields, which agrees with experimental observations. Besides, Anderson-type disorder is also shown to be beneficial in suppressing the dissipation of ρxx. These findings provide useful insight to the design and application of future QAHE devices.

Acknowledgments

This work is supported by the MOST Project of China (2017YFA0303301, No. 2016YFA0300603, No. 2015CB92-1102 and No. 2014CB920903), and the NNSFC (No. 1167-4024, No. 11504240, No. 11574029, No. 11574007).

ORCID iDs

Yanxia Xing https://orcid.org/0000-0002-9010-6583

References

[1] Hasan M Z and Kane C L 2010 Rev. Mod. Phys. 82 3045
[2] Qi X-L, Hughes T L and Zhang S-C 2008 Phys. Rev. B 78 195424
[3] Fu L, Kane C L and Mele E J 2007 Phys. Rev. Lett. 98 106803
[4] Murakami S 2003 Science 301 1348
[5] Bernevig B A, Hughes T L and Zhang S-C 2006 Science 314 1757
[6] Konig M, Wiedmann S, Brune C, Roth A, Buhmann H, Molenkamp L W, Qi X-L and Zhang S-C 2007 Science 318 766
[7] Liu C, Hughes T L, Qi X-L, Wang K and Zhang S-C 2008 Phys. Rev. Lett. 100 236601
[8] Haldane F D M 1988 Phys. Rev. Lett. 61 2015
[9] Qiao Z, Yang S A, Feng W, Tse W-K, Ding J, Yao Y, Wang J and Niu Q 2010 Phys. Rev. B 82 161414
[10] Tse W-K, Qiao Z, Yao Y, MacDonald A H and Niu Q 2011 Phys. Rev. B 83 155447
[11] Ren Y, Zeng J, Wang K, Xu F and Qiao Z 2017 Phys. Rev. B 96 155445
[12] Qiao Z, Han Y, Zhang L, Wang X, Deng K, Jiang H, Yang S A, Wang J and Niu Q 2016 Phys. Rev. Lett. 117 056802
[13] Liu C-X, Qi X-L, Dai X, Fang Z and Zhang S-C 2008 Phys. Rev. Lett. 104 146802
[14] Yu R, Zhang W, Zhang H-J, Zhang S-C, Dai X and Fang Z 2010 Science 329 61
[15] Chang C-Z et al 2013 Science 340 167
[16] Kou X et al 2014 Phys. Rev. Lett. 113 137201
[17] Bestwick A J, Fox E J, Kou X, Pan L, Wang K L and Goldhaber-Gordon D 2015 Phys. Rev. Lett. 114 187201
[18] Chang C-Z, Zhao W, Kim D Y, Zhang H, Assaf B A, Heiman D, Zhang S-C, Liu C, Chan M H W and Moodera J S 2015 Nat. Mater. 14 473
[19] Mani A and Benjamin C 2018 Sci. Rep. 8 1335
[20] Wang J, Lian B, Zhang H and Zhang S-C 2013 Phys. Rev. Lett. 111 086803
[21] Jiang H, Qiao Z, Liu H and Niu Q 2012 Phys. Rev. B 85 045445
[22] Wang J, Lian B, Zhang H, Xu Y and Zhang S-C 2013 Phys. Rev. Lett. 111 136801
[23] Chu R-L, Shi J and Shen S-Q 2011 Phys. Rev. B 84 085312
[24] Xing Y, Xu F, Cheung K T, Sun Q-f, Wang J and Yao Y-g 2018 New J. Phys. 20 043011
[25] Datta S 1995 Electronic Transport in Mesoscopic System (Cambridge: Cambridge University Press)
[26] Shen S-Q 2012 Topological Insulators, Dirac Equation in Condensed Matter Physics (Berlin: Springer)
[27] Lu H-Z, Zhao A and Shen S-Q 2013 Phys. Rev. Lett. 111 146802
[28] Zhang S-F, Jiang H, Xie X C and Sun Q-F 2014 Phys. Rev. B 89 155419
[29] Liu C-X, Qi X-L, Zhang H-J, Dai X, Fang Z and Zhang S-C 2010 Phys. Rev. B 82 045122
[30] Zhang H, Liu C-X, Qi X-L, Dai X, Fang Z and Zhang S-C 2009 Nat. Phys. 5 438
[31] Xing Y, Sun Q-F and Wang J 2009 Phys. Rev. B 80 235411
[32] Xing Y and Sun Q-F 2014 Phys. Rev. B 89 085309
[33] Zhang L, Zhuang J, Xing Y, Li J, Wang J and Guo H 2014 Phys. Rev. B 89 245107
[34] Lopez Sancho M P, Lopez Sancho J M and Rubio J 1981 J. Phys. F: Met. Phys. 14 1205
[35] Lopez Sancho M P, Lopez Sancho J M and Rubio J 1985 J. Phys. F: Met. Phys. 15 851
[36] Lee D H and Joannopoulos J D 1981 Phys. Rev. B 23 4988
[37] Lee D H and Joannopoulos J D 1981 Phys. Rev. B 23 4997
[38] Li J, Chu R-L, Jain J K and Shen S-Q 2009 Phys. Rev. Lett. 102 136806
[39] Xing Y, Zhang L and Wang J 2011 Phys. Rev. B 84 035110