Quantum Anomalous Hall Effect with Higher Plateaus

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Quantum anomalous Hall (QAH) effect in magnetic topological insulators is driven by the combination of spontaneous magnetic moments and spin-orbit coupling. Its recent experimental discovery raises the question if higher plateaus can also be realized. Here we present a general theory for QAH effect with higher Chern numbers, and show by first-principles calculations that thin film magnetic topological insulator of Cr-doped Bi$_2$(Se,Te)$_3$ is a candidate for the $C = 2$ QAH insulator. Remarkably, whereas higher magnetic field leads to lower Hall conductance plateaus in the integer quantum Hall effect, higher magnetic moment leads to higher Hall conductance plateaus in the QAH effect.

The general theory for higher Chern number QAH effect presented in this letter is generic for any thin films of magnetic TIs. We would like to start from a simple model describing TIs Bi$_2$Te$_3$, Bi$_2$Se$_3$ and Sb$_2$Te$_3$ for concreteness [11]. The thin films made out of this family of compounds doped with Cr or Fe develops ferromagnetism even up to 190 K [15,17]. The QAH effect can be realized in 2D thin film of such magnetic TIs with spontaneous FM order. The low-energy bands of these materials consist of a bonding and an antibonding state of compounds $\sigma$-Pauli matrices.

$$H_{3D}(k_x, k_y, k_z) = \begin{pmatrix} H_+(k) & A_1 k_z i\sigma_y \\ -A_1 k_z i\sigma_y & H_-(k) \end{pmatrix},$$

$$H_\pm(k) = \varepsilon(k) + d_\pm^\dagger(k)\tau_i,$$

where $\tau_i$ ($i = 1, 2, 3$) and $\sigma_y$ are Pauli matrices. $d_\pm^\dagger(k) = (A_2 k_x \pm A_3 k_y, M(k) \pm \Delta)$. To the lowest order in $k$, $M(k) = B_0 + B_1 k_z^2 + B_2 (k_x^2 + k_y^2)$, $\varepsilon(k) = D_0 + D_1 k_z^2 + D_2 (k_x^2 + k_y^2)$ accounts for the particle-hole asymmetry. $B_0 < 0$ and $B_1, B_2 > 0$ guarantee the system is in the inverted regime. The basis of Eq. (1) is $|P_1^+\uparrow\rangle, |P_2^+\downarrow\rangle, |P_1^-\downarrow\rangle, |P_2^-\uparrow\rangle$, and the $z$ axis is chosen as the spin up and down states, respectively. $\Delta$ is the exchange field along the $z$ axis introduced by the FM ordering. For simplicity, the same effective $g$-factor for the two orbitals $P_1^+$ and $P_2^-$ is assumed.

The confinement of thin films of three-dimensional (3D) magnetic TIs in the $z$ direction quantizes the momentum on this axis and leads to 2D sub-bands labeled

$$C_{(Bi,Sb)}$$

experimentally discovered in magnetic TI of Cr-doped...
by the sub-band index $n$. In order to illustrate the underlying physics clearly, we first take the limit $A_1 = 0$, in which case the system is decoupled into two classes of 2D models $h_+(n)$ and $h_-(n)$ with opposite chirality

$$\tilde{H}_{2D}(n) = \begin{pmatrix} h_+(n) & 0 \\ 0 & h_-(n) \end{pmatrix}$$

where $h_{\pm}(n) = \tilde{\varepsilon}_n 1_{2\times2} + (\tilde{M}_n \pm \Delta) \tau_3 + A_2k_x\tau_1 \pm A_2k_y\tau_2$, expressed in the subspace of $|E_n, \uparrow\rangle = \varphi_n(z)|P1^+\uparrow\rangle$, $|H_n, \downarrow\rangle = \varphi_n(z)|P2^-\downarrow\rangle$ for $h_+(n)$ and $|E_n, \downarrow\rangle = \varphi_n(z)|P1^-\downarrow\rangle$, $|H_n, \uparrow\rangle = \varphi_n(z)|P2^+\uparrow\rangle$ for $h_-(n)$. $\tilde{\varepsilon}_n = D_0 + D_1(k^2_x)_n + D_2(k^2_x + k^2_y)$, $M_n = B_0 + B_1(k^2_x)_n + B_2(k^2_x + k^2_y)$, and the confinement in a thin film of thickness $d$ is given by the relation $\varphi_n(z) = \sqrt{2/d} \sin(n\pi z/d + n\pi/2)$ and $(k^2_n) = (n\pi/d)^2$ for sub-bands index $n$. $|E_n, \uparrow\uparrow\rangle$ and $|H_n, \uparrow\downarrow\rangle$ have parity $(-1)^{n+1}$ and $(-1)^n$, respectively. At half filling, the effective models $h_{\pm}(n)$ have Chern number $\pm 1$ or $\pm 1$ depending on whether the Dirac mass is inverted ($\tilde{M}_n \pm \Delta < 0$) or not ($\tilde{M}_n \pm \Delta > 0$) at $\Gamma$ point. Thus the total Chern number of the system is

$$C = N_+ - N_-$$

where $N_{\pm}$ is the number of $h_{\pm}(n)$ with inverted Dirac mass, respectively. As shown in Fig. 1(a), when $\Delta = 0$, $N_+ = N_-$, thus the net Hall conductance of this system vanishes; while the $Z_2$ index $N_2$ (mod 2), can be still nonzero, which gives the crossover from 3D TI to quantum spin Hall insulator [13]. When $\Delta \neq 0$, $N_+$ can be different from $N_-$. In the $\Delta = \Delta_1$ case, only the Dirac mass of $h_+(1)$ is inverted, thus $N_+ = 1$ and $N_- = 0$, the system is in a QAH state with $C = 1$. When the exchange field is larger with $\Delta = \Delta_2$, the Dirac mass of $h_-(1)$ and $h_+(2)$ are inverted, $N_+ = 2$ and $N_- = 0$, gives QAH phase with $C = 2$.

With the criteria for the Chern number in Eq. (4), we can identify a phase diagram in the parameter space $(\Delta, d)$ as shown in Fig. 2, where we adopt the parameters of Bi$_2$(Se$_{0.4}$Te$_{0.6}$)$_3$ [14], and neglect the particle-hole asymmetric term $\tilde{\varepsilon}_n$ for it does not change the condition for band inversion. In the absence of $A_1$ term, the condition for band inversion of $h_+(n)$ is $d > n\pi \sqrt{B_1/(\pm \Delta - B_0)}$, thus the phase boundaries are given by $d = n\pi \sqrt{B_1/(\pm \Delta - B_0)}$ [Fig. 2(a)]. The different QAH phases are denoted by the corresponding Chern numbers. As shown in Fig. 2(b), when $A_1$ term is turned on, it induces the coupling between $h_+(n)$ and $h_+(n+1)$, which makes the QAH phases with same Chern numbers simply connected in the phase diagram. Also it enlarges the $C = 1$ phase and shrinks $C = 2$ phase in the parameter space. The phase space of odd Chern number phases are simple connected, while those of even Chern number phases are separated into “islands”, for the confinement potential has inversion symmetry along the $z$ direction.

For a given thickness, the Hall conductance experiences incremental plateaus $0, e^2/h, 2e^2/h, \cdots$ as $\Delta$ increases. Remarkably, the inverse of the magnetization, proportional to $1/\Delta$ in QAH effect, is analogous to the magnetic field in IQHE. One the other hand, for a given exchange field, when the thickness $d$ is small enough, the band inversion in the bulk band structure will be removed entirely by the finite size effect; with the increasing $d$, finite size effect is getting weaker and the band inversion among these sub-bands restores. If $\Delta > |B_0|$, the Dirac mass of class $h_-(n)$ can never be inverted, the Hall conductance plateaus transition always increase as $d$ increases. If $\Delta$ is small, the Dirac mass of the both classes can be inverted, and the system can only oscillate between $C = 1$ QAH insulator and trivial band insulator as a function of thickness. Therefore, the QAH effect with higher plateaus requires a large enough exchange field.

FIG. 1. Evolution of the subband structure upon increasing the exchange field. The solid lines denote the sub-bands that have even parity at $\Gamma$ point, and dashed lines denote sub-bands with odd parity at $\Gamma$ point. The blue color denotes the spin up electrons; red, spin down electrons. (a) The initial $(E_1, H_1)$ sub-bands are already inverted, while the $(E_2, H_2)$ sub-bands are not inverted. The exchange field $\Delta_1$ release the band inversion in one pair of $(E_1, H_1)$ sub-bands and increase the band inversion in the other pair, while the $(E_2, H_2)$ sub-bands are still not inverted. With stronger exchange field $\Delta_2$, a pair of inverted $(E_2, H_2)$ subbands appears, while keeping only one pair of $(E_1, H_1)$ subbands inverted. (b) Schematic drawing of a Hall bar device of $C = 2$ QAH effect, and (c) expected chemical potential dependence of zero magnetic field $\rho_{xy}$ (in red) and $\rho_{xx}$ (in blue).
choose Cr-doped Bi$_2$(Se$_{0.4}$Te$_{0.6}$)$_3$ as an example, where the Dirac cone of surface states is observed to locate in the bulk band gap [19]. Here, we first carried out the first-principles calculations on 3D Bi$_2$(Se$_{0.4}$Te$_{0.6}$)$_3$ without SOC, the virtual crystal approximation is employed to simulate the mixing between Se and Te in first-principles calculations. Then we get the effective SOC parameter of Bi$_{2−y}$Cr$_y$ by fitting the band structure of Bi$_{1.78}$Cr$_{0.22}$(Se$_{0.6}$Te$_{0.4}$)$_3$ in Ref. [19]. This system is at the critical point of the topological phase transition from inverted bands to normal bands, because the substitution of Bi by Cr reduces SOC strength. Finally, we construct the tight-binding model with SOC and the exchange interaction based on maximally localized Wannier functions [20, 21].

When the 2D system stays in the QAH phase, there are topologically protected chiral edge states at the 1D edge. To show the topological feature more explicitly, we calculate the dispersion spectra of the chiral edge states directly. As examples, here we study the edge states of the 6-QLs and 12-QLs of Bi$_{2−y}$Cr$_y$(Se$_{0.4}$Te$_{0.6}$)$_3$ film along [11] direction (Edge A along Γ-M), as shown in Fig. 3. For a semi-infinite system, combining the tight-binding model with the iterative method [22], we can calculate the Green’s function for the edge states directly. The local density of states (LDOS) is directly related to the imaginary part of Green’s function, from which we can obtain the dispersion of the edge states. As shown in Fig. 3(f) for 12-QLs Bi$_{1.78}$Cr$_{0.22}$(Se$_{0.4}$Te$_{0.6}$)$_3$ with $\Delta = 0.14$ eV, there indeed exist two gapless chiral edge states $\Sigma_1$ and $\Sigma_2$ in the 2D bulk gap indicating the $C = 2$ QAH effect.

Recent experiments have shown that the thickness of thin films TIs can be well controlled through layer-by-layer growth via molecular beam epitaxy [23], and the exchange field $\Delta$ can be tuned by changing the doping concentration $y$ of the magnetic elements [15–17]. In the mean field approximation, $\Delta$ can be estimated as $\Delta = yJ_{\text{eff}}(S)/2$, where $(S)$ is the mean field expectation value of the local spin, and $J_{\text{eff}}$ is the effective exchange parameter between local moments and the band electron. For Cr-doped Bi$_2$(Se,Te)$_3$, $(S) = 3/2$, $J_{\text{eff}}$ is around 2.7 eV [9], and the FM Curie temperature is about tens of K. With the concentration of the magnetic dopants to be 10%, the exchange field can be as large as 0.2 eV, making the realization of QAH effect with higher plateaus feasible.

Experimentally, for the QAH effect with a higher Chern number $C$, the gate-tuned Hall resistance $\rho_{xy}$ should be accurately quantized into $h/Ce^2$ plateau at zero magnetic field accompanied by a vanishing longitudinal resistance $\rho_{xx}$ and conductance as shown in Fig. 1(c). In real materials, there always exists residual dissipative conduction channels contributed by a small amount of bulk carriers; however, if the carrier density is low enough, they will become localized states by the disorder potentials and will not affect the exact quantization of...
FIG. 3. Band structure, Brillouin zone and Edge states. (a) Band structure for 12-QLs Bi$_{12}$Cr$_{0.22}$(Se$_0.4$Te$_{0.6}$)$_3$ without exchange field. The dashed line indicates the Fermi level. (b) The top view of 2D thin film with two in-plane lattice vectors $a_1$ and $a_2$. The 1D edges are indicated by the dashed lines, Edge $A$ along [11] direction (blue) and Edge $B$ along [01] direction (red). The inset shows the 2D Brillouin zone, in which the high-symmetry $a$ points $\Gamma(0,0)$, $K(\pi,\pi)$ and $M(\pi,0)$ are labelled. (c)-(f) Energy and momentum dependence of the LDOS along Edge $A$ for the Bi$_{12}$Cr$_{0.22}$(Se$_0.4$Te$_{0.6}$)$_3$ film with thickness of 6-QLs and exchange field 0.0 eV (c), 0.08 eV (d) and thickness of 12-QLs and exchange field 0.08 eV (e), 0.14 eV (f). Here, the warmer colours represent higher LDOS. The red and blue regions indicate 2D bulk energy bands and energy gaps, respectively. The gapless chiral edge states can be clearly seen around the $\Gamma$ point as red lines dispersing in the 2D bulk gap. In (c), (d), (e), (f), the number of chiral edge state is $C = 0, 1, 1, 2$.

The QAH effect with higher plateaus may provide a setting for both fundamental and applied investigation. A wealth of materials with tunable magnetic and topological properties [24, 25] could lead to the discovery of even higher Chern number QAH insulators. The multiple dissipationless edge channels in higher plateau QAH effect would offer better ways to optimize electrical transport properties, leading to novel designs for low-power-consumption electronics.

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