Three-dimensional topological insulator in a magnetic field: chiral side surface states and quantized Hall conductance

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Abstract

Low energy excitation of surface states of a three-dimensional topological insulator (3DTI) can be described by Dirac fermions. By using a tight-binding model, the transport properties of the surface states in a uniform magnetic field are investigated. It is found that chiral surface states parallel to the magnetic field are responsible for the quantized Hall (QH) conductance \((2n + 1)\frac{e^2}{h}\) multiplied by the number of Dirac cones. Due to the two-dimensional nature of the surface states, the robustness of the QH conductance against impurity scattering is determined by the oddness and evenness of the Dirac cone number. An experimental setup for transport measurement is proposed.

1. Introduction

The topological insulator (TI), a new quantum state with an insulating bulk and a metallic surface, has attracted much attention [1] since its theoretical predictions [2–4] and its experimental realizations [5–8] in three dimensions. Unlike normal insulators, the boundary of a finite TI sample supports extended and current carrying states in its bulk gap. In the presence of spin–orbital coupling, which respects time reversal symmetry (symplectic), three-dimensional (3D) TIs can be classified by a \(\mathbb{Z}_2\) invariant integer \(\nu\) [9–12] into a weak TI for even number of the Dirac cones (called \(\nu = 1\)) and a strong TI for odd number of the Dirac cones (called \(\nu = -1\)). The impurity scatterings in strong and weak TIs behave differently [2, 3, 13].

The surface states of a three-dimensional topological insulator (3DTI) are described by two-dimensional (2D) Dirac cones centered at the time reversal equivalent points in the Brillouin zone. 2D Dirac fermions with a single cone are predicted to have many novel properties such as the Klein paradox, anti-localization, etc [14–17]. In the quantum Hall effect (QHE) regime (strong magnetic field), the Landau levels of a single cone Dirac fermion are unevenly distributed

\[ E_n \sim \sqrt{B|n|}, \quad n = 0, \pm 1, \pm 2, \ldots \] (1)

This distribution has been confirmed by several experiments [18–20]. Therefore, for such systems, it is now natural to ask the following questions: is there a quantum Hall effect (QHE) associated with these Landau levels? What would this effect look like and how can we measure it experimentally? This will be the focus of the present work.

In this paper, we investigate a 3DTI in a uniform magnetic field within a well known tight-binding model. Our calculations yield indeed the well known Landau levels (equation (1)). However, the issue of the QH conductance is subtle. All surface states of a finite 3DTI are fully connected with each other [2, 3, 23] and surface states living on the sample surface may move from one side to another. In other words, the well defined Hall voltage measurement in usual 2D electron gases (2DEG) is not so clear in the 3DTI cases.
since two surfaces cannot be separated by the bulk of a finite 3DTI as in 2D QHE systems. The current does not come from 1D edge channels, but from 2D surface states. The structures of these side surface states are more complicated than the edge states in 2DEG or purely 2D Dirac fermion [16, 21, 22]; therefore, well defined quantum Hall plateaus $(2n+1)^2 \pi$ can only be defined from transverse current instead of the traditional Hall voltage. Our tight-binding calculations confirm the earlier predictions based on an effective theory of Dirac fermions in curved 2D spaces [23] and make the effect understood within a band theory picture. The robustness of the Hall conductance against impurities is also studied. Our tight-binding model and its basic properties are introduced in section 2. Numerical results and their discussions are presented in section 3, followed by the conclusion.

2. Model

A well known tight-binding model of 3DTI [24] is

$$H_0(k) = \epsilon_0(k)I_{4\times 4} + \sum_{\alpha = 1}^{5} d_\alpha(k) \Gamma^\alpha$$

$$d_\alpha(k) = (A_2 \sin k_x, A_2 \sin k_y, A_1 \sin k_z, M(k), 0),$$

where $\epsilon_0(k) = C + 2D_1 + 4D_2 - 2D_1 \cos k_x - 2D_2 (\cos k_x + \cos k_y), M = M - 2B_1 - 4B_2 + 2B_1 \cos k_z + 2B_2 (\cos k_x + \cos k_y)$ and $\Gamma^{1, 2, 3, 4, 5} = (\sigma_x \otimes \sigma_x, \sigma_y \otimes \sigma_y, \sigma_y \otimes I_{2 \times 2}, \sigma_x \otimes I_{2 \times 2}, \sigma_0 \otimes s_z)$ in the basis of four states ($|P^z_1, \uparrow\rangle$, $|P^z_1, \downarrow\rangle$, $|P^z_2, \uparrow\rangle$, $|P^z_2, \downarrow\rangle$). After inverse Fourier transformation of equations (2), the real space version of this model on a cubic lattice can be written in the form

$$H_0 = \sum_{is} \epsilon_i c_i^\dagger c_is + \sum_{\langle ij \rangle IS} t_{ij} c_i^\dagger \sigma_i c_j + H.c.,$$

where $i, j$ are lattice site indices, $s \in \{ |P^z_1, \uparrow\rangle, |P^z_1, \downarrow\rangle, |P^z_2, \uparrow\rangle, |P^z_2, \downarrow\rangle \}$ is the spin–orbital index. The first term in equation (3) is the on-site energy; the second and third terms describe the hoppings between nearest neighbor sites. The effect of non-magnetic impurities can be included by adding a term

$$H_1 = \sum_i V_i c_i^\dagger c_i,$$

where $V_i$ distributes randomly in the energy range of $(-W/2, W/2)$. The magnetic field $B$ is introduced through the Peierls substitution of hopping coefficients [25, 26]

$$t_{ij}^\prime = \exp \left( \frac{2\pi i}{\phi_0} \int_i^j dl \cdot A \right) t_{ij},$$

where $\phi_0 = e/h$.

In the clean limit ($H_1 = 0$), this 3D model is fully gapped in the energy range $(-M, M)$. The properties of surface states within this gap are determined by the $Z_2$ topological numbers related to the time reversal polarizations [2, 3, 9]

$$\delta_i = \frac{\sqrt{\det[w(T_i)]}}{|P[T(w(T_i))]|} = -\text{sgn}(d_4(k = \Gamma_i)) = \pm 1,$$

at eight time reversal invariant points in the first Brillouin zone: $\Gamma_1, 2, 3, 4, 5, 6, 7, 8 = (0, 0, 0), (\pi, 0, 0), (0, \pi, 0), (0, 0, \pi), (\pi, \pi, 0), (\pi, 0, \pi), (\pi, \pi, \pi)$, where the matrix $w_{nn}(k) = (u_{k-n}[\theta](\delta_{kn})$. If $\nu = \prod_{i=1}^{8}\delta_i = -1$, the system is a strong 3DTI with odd numbers of the Dirac cones on each surface. Otherwise, the system ($\nu = 1$) is a weak 3DTI with even numbers of the Dirac cones on each surface. In terms of model parameters, the system is in a strong (weak) TI phase when $B_i/M > 1$ ($B_i/M < -1$) [2].

The surface states around each Dirac cone are approximately described by the Dirac fermion Hamiltonian (the $z$-axis is normal to the surface) [4, 16, 24, 27]

$$H_{xy} = v_F (\sigma_k k_y - \sigma_z k_z),$$

with a linear dispersion relation

$$E_{xy} = \pm v_F \sqrt{k_x^2 + k_z^2},$$

where $v_F = A_2 \sqrt{1 - (\frac{D_1}{A_1})^2}$ and $h = 1$ is adopted.

Before presenting calculations of tight-binding models, let us first look at effective model (equation (7)) in a field $B = (0, 0, B)$ perpendicular to the surface. In the Landau gauge $A = (-By, 0, 0)$, $H_{xy}$ is [15]

$$H_{xy} = v_F [\sigma_z (k_y - A_z) - \sigma_y (k_x - A_x)],$$

$$= v_F \begin{pmatrix} k_y - i(k_z + eBy) & 0 \\ 0 & k_z - i(k_x + eBy) \end{pmatrix},$$

where $k_i = -i\partial_i$. The eigenvalues are Landau levels [15]

$$E_{xy} = \pm v_F \sqrt{2neBy}, \quad n = 0, 1, 2, \ldots$$

However, for the surface parallel to magnetic field $B$, say, the $x$–$z$ plane, and in the same gauge $A = (-By, 0, 0)$, the Hamiltonian is

$$H_{xz} = \sigma_y (k_z - A_x) - \sigma_z (k_x - A_x),$$

$$= \begin{pmatrix} 0 & k_z - i(k_x + eBy) \\ k_x + i(k_z + eBy) & 0 \end{pmatrix}.$$ 

Since $eBy$ is a constant for a definite $x$–$z$ plane, and commutes with $k_x$ and $k_z$, the only difference between equations (11) and (7) is a global shift $-eBy$ of the Dirac cone in the $k_z$ direction. The eigenvalue shows

$$E_{xz} = \pm v_F \sqrt{(k_x + eBy)^2 + k_z^2}.$$ 

Although equation (12) appears to be dependent on $y$ (thus also on the reference point and gauge) when the eigenstates are labeled by $k_x$ and $k_z$ for a given $y$, $E_{xz}$ will not explicitly depend on $y$ if one uses new labels of $k_x'$ defined as $k_x' = k_z + eBy$ and $k_z$. In other words, the eigenenergies of the system, or spectrum, are independent of the choice of gauge and reference point except for a global shift in $k$ space. The only difference is that Dirac cones for different $y$ center at different ($k_x = -eBy$, $k_z = 0$). For example, for the energy spectrum of the front surface ($y = 1$) of an $N_x \times N_y \times N_z$ sample, the Dirac cone centers at $(k_x, k_z) = (-eB, 0)$ while that for the back surface ($y = N_y$) centers at $(k_x, k_z) = (-eBN_y, 0)$.
The criterion of this transition is marked by the ratio of sample size. Fermion physics instead of the massless one mentioned. The points are opened [28–30]. Then one has a massive Dirac on both sides will couple together and gaps around the Dirac in numerical simulations and even real experiments. If the discuss the finite-size effects of 3DTI that might be important physical observations are independent of the global shifts of the dispersion curves associated with the different choices of gauge and y-coordinate. We shall see that states in the surfaces parallel to the magnetic field play an important role in the QHE in 3DTI.

3. Numerical results

To be specific, we consider Hamiltonian (3) on a cubic lattice with size $N_x \times N_y \times N_z$. For a slab $\infty \times \infty \times N_z$ of thickness $N_z$ in the z-direction and infinite in other two directions [3], the surface states of the TI can be displayed by plotting the dispersion relation $E(k_x, k_z)$ inside the bulk gap so that this dispersion relation must be from the surface states. Figure 1(a) is the dispersion relation of a slab without a magnetic field. The Dirac cone can be clearly seen. There are two degenerated Dirac cones located on lower ($z = 1$) and upper ($z = N_z$) surfaces, respectively. The existence of such surface states is rooted in the topological property of time reversal symmetric systems [2, 9].

Before continuing our presentation, we would like to discuss the finite-size effects of 3DTI that might be important in numerical simulations and even real experiments. If the distance between opposite surfaces is too small, surface states on both sides will couple together and gaps around the Dirac points are opened [28–30]. Then one has a massive Dirac fermion physics instead of the massless one mentioned. The criterion of this transition is marked by the ratio of sample size and the decay depth of the surface states. For our model here, the decay depth is [30]

$$
\xi_0(E) = \sqrt{\frac{2(D_1^2 - B_1^2)}{-F + (-1)^{\alpha} - 1/\sqrt{R}}},
$$

(13)

where $F = A_1^2 + 2D_1(E - C) - 2B_1M$ and $R = F^2 - 4(D_1^2 - B_1^2)[(E - C)^2 - M^2]$, and the index $\alpha$ labels the two independent solutions. For the model parameters we adopt in figure 1, Re($\xi$) $\approx$ 1.5 in units of lattice constants. Therefore it is safe to say that the finite-size effects in our calculations are practically avoided.

The magnetic field breaks time reversal symmetry and the fate of surface states will be tested in the following tight-binding calculation. A uniform magnetic field generally also breaks the lattice translational symmetry [31] and results in the Hofstadter butterfly spectrum [32]. If the magnetic flux through a unit cell is a fraction of the flux quanta, $B\alpha^2 = \frac{2}{\Phi_0}$, where $p$ and $q$ are two prime numbers and $a$ is the lattice constant, periodic structure is restored with an enlarged and y-elongated unit cell of $q$ times of the original one, $a'_x = a_x$ and $a'_y = qa_y$, then $k_x \in [-\pi/a, \pi/a]$ and $k_y \in [-\pi/(qa), -\pi/(qa)]$ are still good quantum numbers [33, 34]. Figure 1(b) is the dispersion relation of the same slab as that for figure 1(a) in a perpendicular magnetic field $B = (0, 0, B)$. Instead of a linear dispersion relation in zero field, discrete Landau levels $E_n$ appear. We have confirmed that there is an upper–lower surface double degeneracy and all wavefunctions are strongly confined inside (top/bottom)
surfaces. Although the time reversal symmetry is broken, the magnetic field does not destroy the 2D nature of the surface states. The dependence $E_0 \sim \sqrt{n}$ is also verified as shown in the inset of figure 1(b). Such Landau levels have already been observed in recent experiments [19, 20].

We also plot the dispersion relation for the infinite $x$-$z$ surfaces associated with the strong TI lattice $N_x \times N_z \times N_y = \infty \times N_z \times \infty$ in a parallel magnetic field $B = (0, 0, B)$ in figure 1(c). Shifted Dirac cones corresponding to two surfaces ($y = 1$ and $N_y$) can be clearly seen, as predicted in equation (12). However, the corresponding dispersion relations are the same, except for a global shift of $k_x$ coordinate, $k_x' = k_x - eBy_0$. We shall see that these side surface states play an important role in the following discussion. Figure 1(d) is similar to (c) when the infinite surface is confined along the $z$-direction with a periodic boundary condition that eliminates possible edge states. Subband structures appear due to the $z$-confinement.

With quantized Landau levels, one naturally expects quantum Hall effects. In conventional 2DEGs, quantized Hall conductance comes from the spatially separated counter-propagating edge channel(s) on the two sides of a sample [35]. The situation in 3D is subtle because a surface state may cover all surfaces because they are fully connected [2, 3, 23]. In other words, a surface state cannot be confined on only one surface, resulting in more interesting and richer physics.

To study possible current carrying surface states, we consider a bar geometry of finite widths of $N_y$ and $N_z$ in both $y$- and $z$-directions. The dispersion relation along the $x$-direction in a magnetic field is plotted in figure 2. The constant energy in the middle of the curves shows that the Landau levels exist in the middle of the surface. The Landau levels float up near the edges (junctions of two surfaces). We have confirmed that the left-most ($k_x < 0.1$) and right-most ($k_x > 0.8$) parts of the curves correspond to states distributed mostly on the left ($y = 1$) and the right ($y = N_y$) side surfaces, respectively (figure 3). These side surface states are spin polarized due to spin–orbit coupling [23], as plotted in figure 4.

As illustrated in figures 3(a)–(e), varying $k_x$ from either side of the curves to the middle flat parts, the states move from the side surfaces of $y = 1$ and $N_y$ (figure 1(d)), to the top and bottom surfaces of $z = 0$ and $N_z$ (figure 1(b)) continuously. This is possible because a particle can move from the side surfaces to the top/bottom ones without passing through the bulk. In other words, the surface states live essentially on a closed surface of a finite 3DTI sample. One cannot have 1D edge channels as in the 2D case. The discreteness of these states simply originates from the finite thickness $N_z$ in the $z$-direction, as indicated in figures 2(a) and (b). Increasing $N_z$ does not affect the Landau levels, but generates more side surface-state subbands. In the limit of large $N_z$, these subbands pack densely and form two continuum cones, similar to the shifted Dirac cones in parallel magnetic field in figure 1(c).

Similar to edge states in conventional 2D systems, due to non-zero dispersion, the side surface states can transport electrons in the presence of voltage along the $x$ direction. The effects of side surface states have been noticed in a recent transport measurement [36]. However, the side surface states are quite different from the edge states in 2DEG. For example, the dependence of $E_0(k_x)$ is non-monotonic on each side. This brings the coexistence of both forward and backward moving channels on each side, as illustrated in figure 5. At each side and for a given energy, the numbers of forward moving channels ($n_f$) and backward moving ones ($n_b$) depend on magnetic field $B$, as well as thickness $N_z$ of the sample. However, their difference $n_f - n_b = 1, 3, 5, \ldots$ is universal between any definite pair of adjacent Landau levels, since an increase of $n_f$ by one will lead to an increase of $n_b$ by one at the same time. This is valid as long as the dimension of the sample is not too small to couple states on any opposite surfaces [27]. A general theorem guarantees the existence of current carrying states [37]. The directions of these net currents on two sides are reversed, thus they are chiral. Experimentally, such chiral currents can be measured by a multi-terminal measurement illustrated in figure 6. In such setups, the Landauer–Büttiker formula is $I_j = \sum_i T_{ji} - V_j$, where $T_{ji}$ is the transmission from lead $i$ to lead $j$ and $V_j$ are the voltage and the current in the $j$th lead respectively, satisfying Kirchhoff’s law $\sum_i I_i = 0$ [38]. In the clean limit, all the active channels are perfectly conducting.
Figure 3. Spatial distributions of wavefunctions on the y–z section of the bar for the states marked as red dots in figure 2(a). The magnetic field is in the z-direction. (a)–(e) correspond to state points a–e, respectively.

Figure 4. Spatial distributions of local spin $s_z$. (a) and (b) correspond to state points a and b in figure 2, respectively.

and the transmission $T_{j\leftarrow i}$ can be read directly from the profile of the active surface channels, as shown in figure 6. For the four-terminal setup illustrated in figures 6(a) and (b), straightforward calculations within this formalism give

$$G_{xy} = \frac{I_3 - I_4}{V} = \frac{2I_3}{V} = -\frac{2I_4}{V} = (n_f - n_b) \frac{e^2}{h},$$  \hspace{1cm} (14)

$$G_{xx} = \frac{I_1 - I_2}{V} = \frac{2I_1}{V} = -\frac{2I_2}{V} = (n_f + n_b) \frac{e^2}{h}. \hspace{1cm} (15)$$

This $G_{xy}$ is the Hall conductance in the present problem. This is consistent with the previous calculation based on an effective model in curved space [23], but here understood within simple band theories. Similar results hold for the case of surface states with more than one Dirac cone and the only difference is that the conductance is multiplied by a factor of $N_{cone}$, the number of Dirac cones. However, for a 3D six-terminal setup, shown in figure 6(c) and generalized from the traditional 2D Hall bar, similar calculations show that

$$G_{xy} = \frac{V_3 - V_4}{I_1} = \frac{n_b - n_f}{n_b^2 - n_b n_f + n_f^2} \frac{e^2}{h},$$ \hspace{1cm} (16)

$$G_{xx} = \frac{V_5 - V_3}{I_1} = \frac{n_b n_f}{n_b^2 + n_f^2} \frac{e^2}{h}, \hspace{1cm} (17)$$

which is generally sample dependent and no quantized.

One question arises: is the value of the Hall conductance $G_{xy}$ defined in equation (15) robust against disorder [39]? In zero magnetic field, it is well known that the surface states are robust for odd $N_{cone}$ (strong TI) and not for even $N_{cone}$ (weak TI). Since charge transport is dominated by the side surface states at zero field, it is reasonable to expect that the robustness of $G_{xy}$ is also determined by the evenness and oddness of $N_{cone}$. Specifically, for strong TI with single cone
Figure 5. Schematic drawing (seen from above) of the active side surface channels at the Fermi energies $E_1$ (a) and $E_2$ (b) indicated by the orange lines in figure 2(a). The channel numbers of forward moving $n_f$ and backward moving $n_b$ are indicated.

Figure 6. The schematic drawing of 3D multi-terminal measurements of the TI (gray). The uniform magnetic field $B$ (red) is in the $z$-direction. The orange arrows represent the side surface channels that carry currents. (a) The 3D schematic diagram of a four-terminal measurement. A voltage $V$ is applied to the left (1) and right (2) terminals. The potential of the front and back terminals are $V/2$ and $V/2$, respectively. (b) The vertical view of (a) from above. (c) The vertical view of a 3D six-terminal measurement, which is not preferred in our model.

Figure 7. Hall conductance $G_{xy}$ as a function of the Fermi energy $E$ for various disorder strengths $W$. $G_{xy}$ for a strong (a) and weak TI (b) is calculated from a four-terminal setup as illustrated in figure 6. The sample size is $38 \times 18$ and the model parameters are $A_1 = A_2 = 1, B_2 = 1, C = 0, D_1 = D_2 = 0, M = 0.8$ and $B_1 = \pm 1$ for strong (weak) TI.

Surface states in a magnetic field, as illustrated in figure 2, forward and backward channels coexist on the same side, but they originate from a single Dirac cone and the backscattering is small. These are confirmed by numerical simulations of a four-terminal setup as shown in figure 7(a) for a strong 3DTI and in figure 7(b) for a weak 3DTI, by using the standard method of non-equilibrium Green's functions [38, 40]. In the weak TI case, the conductance $G_{xy}$ is twice as large due to double cone degeneracy. Also, its value is sensitive to disorder because of the inter-scattering between the two cones. Since a four-terminal numerical simulation is very resource consuming, in figure 7 we use a smaller system. The physics remains the same as long as there is no direct coupling between surface states on two opposite surfaces [28–30], as stated earlier. Quantized Hall plateaus predicted from the above analysis, especially for the strong TI, can be clearly seen. In the presence of disorder, the quantum Hall plateaus of a strong TI (figure 7(a)) survive much better than those of a weak TI (figure 7(b)).

4. Summary

Before ending this paper, it should be emphasized that we did not obtain the half conductance predicted by a 2D Dirac
fermion effective theory of a single plane [16, 21, 22]. In a less strict sense, we saw the sum of half conductance from upper and lower surfaces [23], since the Dirac fermion lives on a closed and curved surface of 3DTI. By making an edge channel on one surface, one inevitably makes a new one on the opposite surface so that a Dirac fermion will not terminate nowhere on a surface. The exact Hall conductance of one surface cannot directly be observed unless the surface state can be effectively confined in one isolated plane by some means. On the other hand, the quantized Hall conductance we obtained from the 2D surface states should not be viewed as a trivial application of Chern number theory of a 2DEG [33, 34], since the surface states live on a closed 2D manifold embedded in a 3D space, which is topologically different from the 2D plane of a 2DEG.

In summary, we investigated the quantum Hall effect of a 3DTI in a magnetic field. The integer Hall conductance is carried by side surface states due to the non-separable nature of surface states enclosing the 3DTI. The quantum Hall conductance reflects the properties of side surface states that are parallel to the magnetic field. The quantum Hall effect thus offers a transport measurement to determine the topological property of a 3DTI: whether it is a weak or strong TI, the number of Dirac cones, etc.

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