Two-dimensional topological insulators and their edge states

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Abstract. Topological insulators are nonmagnetic insulators in the bulk, but have gapless edge/surface states characterized by $\mathbb{Z}_2$ topological numbers. In this paper we review basic properties of topological insulators. We then focus on the two-dimensional topological insulators, and describe various properties of the edge states.

1. Introduction
Topological insulators (quantum spin Hall systems) are new quantum states theoretically proposed in [1, 2, 3, 4, 5], and then have been experimentally observed by various ways. They are nonmagnetic insulators in the bulk, but have gapless edge/surface states. They can be realized in two dimensions (2D) (Fig. 1(a)) and in three dimensions (3D) (Fig. 1(b)). In the topological insulators, the time-reversal symmetry is assumed, i.e. nonmagnetic. The edge/surface states consist of pairs of states which have opposite spins and propagate in the opposite directions; they are degenerate by the Kramers theorem, and form pure spin currents as has been discussed in the context of spin Hall effect [6, 7].

Any nonmagnetic insulators are classified into either topological insulators or ordinary insulators by using $\mathbb{Z}_2$ topological numbers, which will be discussed in the next section. In the 2D topological insulators, the $\mathbb{Z}_2$ topological number $\nu$ can take two values: $\nu = 1$ for the topological

![Figure 1](image-url)

Figure 1. Schematic figures for (a) a 2D topological insulator and (b) a 3D topological insulator.
insulator, and \( \nu = 0 \) for the ordinary insulator. Nonmagnetic insulators without the spin-orbit coupling are ordinary insulators, and when the spin-orbit coupling becomes stronger, insulators may become topological insulators. Hence, the edge/surface states of topological insulators arise from the spin-orbit coupling. Roughly speaking the mechanism for the emergence of topological insulators from the spin-orbit coupling is the following. The spin-orbit coupling acts as a “spin-dependent magnetic field”, and it gives rise to spin-dependent quantum Hall effect [2, 3]. The edge states from this spin-dependent quantum Hall effect consist of counterpropagating states with opposite spins.

These edge/surface states are called “helical”. They are degenerate due to the Kramers theorem, and these degenerate pairs of states are called Kramers pairs. The important point for these helical edge/surface states is that any time-reversal-symmetric perturbation, such as nonmagnetic impurities or electron-electron interaction, cannot open a gap [8, 9]. This can be understood in the following way: the \( Z_2 \) topological number cannot change continuously when nonmagnetic perturbation is added, and the system remains the topological insulator, even in the presence of perturbation. This robustness of topological insulator against perturbations is called topological protection.

2. Topology and topological insulators

Not all materials with strong spin-orbit coupling are topological insulators; in order to distinguish between topological and ordinary insulators, one has to calculate the \( Z_2 \) topological numbers [2, 10]. First we introduce time-reversal invariant momenta (TRIM), as the momenta satisfying \( k \equiv -k \pmod{G} \), where \( G \) is a reciprocal lattice vector. In the two-dimensional Brillouin zone, there are four TRIM \( k = \frac{1}{2} (n_1 b_1 + n_2 b_2) \), \( (n_1, n_2 = 0, 1) \), where \( b_1 \) and \( b_2 \) are the reciprocal primitive vectors. Let \( k = \Gamma_i \) \( (i = 1, 2, 3, 4) \) denote the four TRIM. Here we explain how to calculate the \( Z_2 \) topological number for inversion-symmetric systems. In this case the Bloch Hamiltonian \( H(k) \) satisfies \( PH(k)P^{-1} = H(-k) \), where \( P \) is the inversion operator (parity). Therefore, at the TRIM \( \Gamma_i \), \( PH(\Gamma_i) = H(\Gamma_i)P \) is satisfied, and the eigenstates at TRIM \( \Psi(\Gamma_i) \) is an eigenstate of \( P \): \( P \Psi(\Gamma_i) = \xi \Psi(\Gamma_i) \). Because \( P^2 = 1 \), the parity eigenvalue \( \xi \) is either \( \xi = 1 \) (symmetric) or \( \xi = -1 \) (antisymmetric).

Let us pick up one TRIM \( k = \Gamma_i \), and consider the product of all parity eigenvalues of Kramers pairs below the Fermi energy:

\[
\delta_i = \prod_{m=1}^{N} \xi_{2m}(\Gamma_i),
\]

where \( \xi_m(\Gamma_i) \) denotes the parity eigenvalues of the \( m \)-th eigenstate from the lowest energy states at \( k = \Gamma_i \). The \( (2m-1) \)-th and \( (2m) \)-th states are Kramers degenerate and share the same parity eigenvalues: \( \xi_{2m-1}(\Gamma_i) = \xi_{2m}(\Gamma_i) \). As a result the \( Z_2 \) topological number \( \nu \) in 2D is expressed as a product of these indices \( \delta_i \) \( (i = 1, 2, 3, 4) \) over the four TRIM:

\[
(-1)^\nu = \prod_{i=1}^{4} \delta_i.
\]

If this expression is +1, it gives \( \nu = 0 \) and it is an ordinary insulator; otherwise, when it is -1, it gives \( \nu = 1 \) and it is a topological insulator.

To illustrate the differences of edge states between ordinary and topological insulators, we consider a semiinfinite plane of a 2D system. The translational symmetry along the boundary of the semiinfinite plane (edge) is assumed, thereby the Bloch wavenumber \( k \) along this direction is a good quantum number. Schematics for the edge states of the ordinary insulators and topological insulators are shown in Fig. 2(a) and (b), respectively. We can see the difference
Figure 2. Schematic figure of edge states for (a) 2D ordinary insulator and (b) topological insulator. (c) Backscattering is prohibited for edge states of 2D topological insulators. (d) Dirac cone of the surface states of 3D topological insulators.

how the edge states are connected to bulk valence or conduction bands. In ordinary insulators the both sides of the edge-state dispersion are connected to the same bulk bands, whereas in topological insulators the edge-state dispersion connects between the bulk conduction and bulk valence bands. We note that because of the spin-orbit coupling, the edge states are spin-split in Fig. 2(a)(b), which is called the Rashba splitting. From the time-reversal symmetry, the edge states which are symmetric with respect to \( k = 0 \) are Kramers degenerate, and have opposite spins. It is noted that Figs. 2(a) and (b) cannot be deformed into each other continuously, without closing the bulk gap. This is guaranteed when the time-reversal symmetry is preserved, and it is a manifestation that these two insulators belong to different topological phases.

Figures 2 (a) and (b) are the simplest cases, and we can consider other types of edge states. Any cases of edge states in nonmagnetic insulators can be classified either into ordinary or topological insulators, by counting the number of Kramers pairs of edge states on the Fermi energy. Even and odd numbers of Kramers pairs correspond then to the ordinary insulators \((\nu = 0)\) and topological insulators \((\nu = 1)\), respectively [10]. In Fig. 2(a), the number of pairs is either two or zero, depending on the value of the Fermi energy within the gap, and in (b) it is one. Thus (a) belongs to the ordinary insulator and (B) does to the topological insulator, in accordance with the previous explanations. This topological number \( \nu \) will not change under continuous change of parameters, unless the bulk gap closes. When the bulk gap closes at some point, the topological number may change. One can classify how the bulk gap closes by changing parameters, and can associate this classification with the change of the topological number [11, 12]. As a result, universal phase diagrams between the topological and ordinary insulators have been found [13].

Here we briefly mention the 3D topological insulators. One of the typical form of surface states of the 3D topological insulators is the single Dirac cone. On the (111) surface of Bi\(_2\)Se\(_3\) or Bi\(_2\)Te\(_3\), the surface Fermi surface is a single Fermi surface encircling the \( \Gamma \) point. The surface-state dispersion is linear in the wavenumber, schematically shown in Fig. 2(d). This is called
a Dirac cone. In Bi$_2$Se$_3$ and Bi$_2$Te$_3$ [14, 15, 16, 17], the surface states observed in experiments form a single Fermi surface around the $\Gamma$ point, and these surface states form a single Dirac cone (Fig. 2(d)).

3. Transport on Edge states of 2D topological insulators
In the edge-state dispersion of topological insulators in Fig. 2(b), we note that the slope of the edge-state dispersion corresponds to the electron velocity $v = \frac{1}{\hbar} \frac{\partial E}{\partial k}$. Therefore, the two edge states in Fig. 2(b) are propagating in the opposite directions, and have the opposite spins due to the time-reversal symmetry. Thus these edge states carry pure spin current [6, 7]. The edge states have fixed velocity directions for each spin. Therefore, nonmagnetic impurities cannot flip spins of the edge-state electrons and hence they cannot backscatter edge states (see Fig. 2(c)). [8, 9]. As a result the edge states form perfectly conducting channels.

These perfectly conducting channels of edge states have been observed in CdTe/HgTe/CdTe quantum well [18, 19, 20]. The CdTe/HgTe/CdTe quantum well was theoretically proposed to be a 2D topological insulator [21] in 2007. This prediction is based on the special band structure of HgTe; due to the strong spin-orbit coupling, HgTe has an inverted band structure, and the gap is zero at the $\Gamma$ point. Because the gap is zero, HgTe itself is not a topological insulator. To open a gap, one should break the cubic symmetry because the degeneracy between the valence and the conduction bands at the $\Gamma$ point is protected by the cubic symmetry. Indeed the gap is opened by making it into a quantum well with CdTe. Detailed calculations show that the system will be a topological insulator when the well thickness $d$ exceeds $d_c = 60 \text{Å}$ [21]. If the well thickness $d$ is less than $d_c$ it is an ordinary insulator. These predictions have been verified in transport experiments. When the Fermi energy is in the bulk band gap, there are no conducting channels for $d < d_c$ and two conducting channels for $d > d_c$. Hence the conductance is predicted to be $G = 2e^2/h$ for $d > d_c$ and $G = 0$ for $d < d_c$, which has been observed in experiments [18, 19]. These perfectly conducting channels has further been verified by nonlocal transport measurements in multiterminal geometry [20].

These perfectly conducting channels can contribute also to thermoelectric transport. In fact, there is an interesting overlap between topological insulator materials and efficient thermoelectric materials. To clarify the reason for this overlap, the thermoelectric transport has been calculated for various cases of special boundary states, such as edge states of 2D topological insulators [22], surface states of 3D topological insulators [23], and helical states on the dislocations [24] of 3D topological insulators [25]. For the edge states of 2D topological insulators [22] or the dislocation states of the 3D topological insulators [25], the electrons do not undergo elastic backscattering, which is good for thermoelectric transport. Nevertheless, in finite temperatures the inelastic scattering causes decoherence of these 1D helical states, and the otherwise good thermoelectric transport will be reduced. It is therefore predicted that at lower temperature, such helical 1D states become gradually dominant over the transport by the bulk carriers, and thermoelectric figure of merit increases.

4. Penetration depth of edge states
To measure or to control the edge states, we should note that the edge states have a finite penetration depth $\ell$ to the bulk. It sets the critical system size, below which the edge states from the both sides of the sample will hybridize and open a gap. To see the penetration depth, previous works used the ribbon geometry [28], where the sample has a finite width in one direction and is infinite in the other direction. In this approach, however, the penetration depth is expressed as a solution of transcendental equation, from which it is difficult to see generic behavior of the penetration depth. Instead we employ the semiinfinite plane, i.e. the $y \leq 0$ region in the $xy$ plane. From this we can get a closed simple formula for the penetration depth $\ell$ [27], and can discuss generic properties of the penetration depth $\ell$. 

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For the calculation we use the following Hamiltonian for the HgTe quantum well.

$$\mathcal{H}(k, k_y) = \begin{pmatrix} H(k) & 0 \\ 0 & H^*(-k) \end{pmatrix},$$

(3)

where $H(k) = \epsilon(k)1 + d^\dagger(k) \sigma^\alpha$, $1$ is a $2 \times 2$ unit matrix, $\sigma^\alpha$ the Pauli matrices, $\epsilon(k) = C - D \left( k_x^2 + k_y^2 \right)$, $d^\dagger = A k_x$, $d^\dagger = A k_y$, and $d^\dagger = M(k) = M - B \left( k_x^2 + k_y^2 \right)$. The eigenenergies are given by $C - Dk^2 + |d(k)|$, and the bulk gap at $k = 0$ is given by $2M$. For calculation on the semiinfinite plane $y \leq 0$, we replace $k_y$ by $-i\partial_y$, and put the boundary condition for the wavefunction to vanish at $y = 0$. Then the allowed eigenstates for the surface states will be the linear combination of the states proportional to $e^{i\lambda y}$ (Re$\lambda > 0$). The detailed calculation in [27] show that there are two allowed values for $\lambda$, which we call $\lambda_1$ and $\lambda_2$. The resulting wavefunction is proportional to $e^{i\lambda_1 y} - e^{i\lambda_2 y}$, where $\lambda_1, \lambda_2 = N \pm \sqrt{N^2 + (k_x - k_x^+)(k_x - k_x^-)}$, and $N = A/(2\sqrt{B^2 - D^2})$. $k_x^\pm$ denote the wavenumbers where the edge-state dispersion is absorbed into the bulk bands. For the parameters of HgTe quantum well, for example, $\lambda_1$ and $\lambda_2$ are real and positive. Because $\lambda_1 > \lambda_2$, as we go from the edge ($y = 0$) into the bulk, the wavefunction proportional $e^{i\lambda_1 y} - e^{i\lambda_2 y}$ rapidly increases within the length $\lambda_1^{-1}$ and then will decrease gradually in the length scale $\lambda_2^{-1}$. Therefore the penetration depth $\ell$ is given by $\ell^{-1} = \lambda_2 = N - \sqrt{N^2 + (k_x - k_x^-)(k_x - k_x^+)}$. Its behavior as a function of wavenumber $k$ is schematically shown in Fig. 3(a). Along the edge-state dispersion, when the wavenumber $k$ approaches the bulk band, the penetration depth $\ell$ diverges, which is naturally expected. In the middle of the edge-state dispersion, the penetration depth $\ell$ becomes minimum, and it is shorter when $k_x^+ - k_x^-$ is larger, i.e. when the edge state extends in a larger region in $k$.

**Figure 3.** (a) Penetration depth $\ell$ for the effective model in the semiinfinite plane. CB (VB) denotes the bulk conduction (valence) band. (b) Penetration depth of the edge states on the zigzag edge of the Bi(111).

By extending this discussion, one can expect that when the dispersion extends over a wider range in $k$, the penetration depth in the middle of the bulk gap becomes larger. One example is the bismuth (111) bilayer film proposed by the author [26, 27]. We show in Fig. 3(b) the band structure for the zigzag edge and the penetration depth of edge states. As we can see, the edge-state dispersion extends over most of the Brillouin zone. Correspondingly, at the middle
of the gap, the penetration depth becomes as short as a few lattice constants. From Fig. 3(b), the edge states consists of three Kramers pairs, and two-terminal conductance is predicted to be $G = 3 \cdot \frac{2e^2}{h} = \frac{6e^2}{h}$ [27].

5. Summary

Topological insulators belong to the class of topological phases as quantum Hall systems do. It is surprising that such topological phases can be realized in zero magnetic field, by the spin-orbit coupling only. The close interaction among theory, experiment, and first-principle calculations is strongly supporting the rapid progress in the field of topological insulators in these several years. In the coming years, we can also expect more discoveries and surprises in this field of topological insulators.

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