Disorder effect in two-dimensional topological insulators

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Abstract. We conduct a systematic study on the disorder effect in two-dimensional (2D) topological insulators by calculating the $Z_2$ topological invariant. Starting from the trivial and nontrivial topological phases of the model describing $HgTe/CdTe$ quantum wells (QWs), we introduce three different kinds of disorder into the system, including the fluctuations in the on-site potential, the hopping amplitude and the topological mass. These kinds of disorder commonly exist in $HgTe/CdTe$ QWs grown experimentally. By explicit numerical calculations, we show that all three kinds of disorder have the similar effect: the topological phase in the system is not only robust to them, but also can be brought about by introducing them to the trivial insulator phase. These results make a further confirmation and extendability of the study on the interplay between the disorder and the topological phase.

1. Introduction
Now topological insulator is the research focus in the field of condensed matter physics[1, 2, 3]. It has an insulating bulk gap and gapless edge or surface states. These gapless states are topologically protected and are immune to nonmagnetic disorder. Recently, in a remarkable development, it has been found that a phase similar to the topological insulator can be brought about by introducing nonmagnetic disorder into a trivial insulator with strong spin-orbit coupling. This new topological phase, referred to as topological Anderson insulator (TAI), has been theoretically predicted in both two- and three- dimensions[4, 5]. A theory based on the self-consistent Born approximation (SCBA) attributes the physics of the TAI phase to the disorder-induced renormalizations of the topological mass and Fermi level[6].

Similar to the topological phases in the clean systems, the TAI phase has a disorder-induced insulating bulk and topologically protected gapless state on the edge. However the edge states cannot be distinguished from the energy spectrum of the disordered systems due to the fact that the localized states may also exist in the gap. So the transport calculations are naturally used to study the extended edge states which contribute a quantized conductance $2e^2/h$ in the two-terminal setup. Since the topological phase can usually be characterized by an invariant, an alternative way to study the TAI phase is to calculate the $Z_2$ topological invariant which is
used to describe time-reversal invariant insulators[7]. In this paper, we conduct a systematic study on the disorder effect in 2D topological insulators by calculating the $Z_2$ topological invariant. Besides the Anderson-type disorder, we also study the effect of disorders in the hopping amplitude and the topological mass. This study may serve as a further confirmation of the existing results and extendability of the study on the interplay between the disorder and the topological phase.

2. The model and method

We start on a model describing $HgTe/CdTe$ QWs. It resides on a square lattice with four orbit states $|s,\uparrow\rangle, |p_x+ip_y,\uparrow\rangle, |s,\downarrow\rangle, |p_x-ip_y,\downarrow\rangle$ (\uparrow, \downarrow denote the electron's spin) on each site. In the momentum space, the Hamiltonian writes[3],

$$H_0(k) = [4D - 2D(cos k_x + cos k_y)]I + [M + 4B - 2B(cos k_x + cos k_y)]\sigma_z + 2A \sin k_x \sigma_x + 2A \sin k_y \sigma_y$$

Here $\sigma$ and $\bar{s}$ are Pauli matrices representing the orbits and the electron’s spin and $I$ is identity matrix. $A, B, D$ and $M$ are four independent parameters. The tight-binding Hamiltonian can be directly obtained by a lattice regulation of the effective low-energy Hamiltonian describing the physics of $HgTe/CdTe$ QWs. We can also view it as a simple toy model conveniently describing both topological and ordinary phases of non-interacting electrons in 2D. The energy spectrum of $H_0(k)$ has two double degenerate branches $E_k = (4D - D_k) \pm \sqrt{(2A \sin k_x)^2 + (2A \sin k_y)^2 + (M - B_k)^2}$, where $\tilde{M} = (M + 4B)$, $B_k = 2B(cos k_x + cos k_y)$ and $D_k = 2D(cos k_x + cos k_y)$. At half-filling, depending on the values of $M$ and $B$, the system can be topological or trivial insulator.

In 2D, the topological invariant is characterized by one $Z_2$ number $\nu$, which distinguishes topological and trivial insulators[2]. Usually it is a difficult problem to evaluate them for a given band structure. However in the presence of inversion symmetry, the problem can be greatly simplified. It has been shown that they can be determined from the knowledge of the parity $\xi_{2m}(\Gamma_i)$ of the $2m$-th occupied energy band at the four time-reversal invariant momenta (TRIM) $\Gamma_i$ that satisfy $\Gamma_i = \Gamma_i + \mathbf{G}$. The four TRIM can be expressed in terms of primitive reciprocal lattice vectors as $\Gamma_i = (n_1b_1 + n_2b_2)/2$, with $n_1 = 0, 1$. Then $\nu$ is determined by the product $(-1)^\nu = \prod_{n_j = 0,1} \delta_{n_1n_2}$, where the parity product for the occupied bands $\delta_i = \prod_{n_m=1}^N \xi_{2m}(\Gamma_i)$.

In the presence of disorder, the system is out of translation invariant symmetry and the above method has to be generalized. It has been known that in the integer quantum Hall effect the invariant can be calculated by introducing generalized periodic boundary conditions and averaging over different boundary condition phases. In fact such considerations are equivalent to take the system as a super-cell of an infinite system[8]. Since the infinite system which is periodic in the super-cell has translation symmetry, the wave vectors can be well defined, which actually corresponds to the boundary condition phases. Under such considerations we recover the band structure, thus we can use the known methods to calculate the topological invariant for the infinite system. The finite system we are studying, which is a super-cell of the infinite system, shares the same topological properties existing in the infinite system. In the following we will apply this method to study the disorder effect of the system. Also to take advantage of the simplification, we only consider disorder configurations with inversion symmetry. Basically such consideration won’t change the underlying physics when the system is big enough. So with this additional symmetry, we only need to consider the Hamiltonian at the four TRIM and they are equivalent to those of a finite system with boundary conditions which are periodic up to phases $\phi_x, \phi_y = 0$ or $\pi$ for boundary sites.
3. The numerical results

Firstly we consider the effect of Anderson-type disorder. It is described by a random on-site potential \( \sum_j U_j \Psi_j^\dagger \Psi_j \) with \( U_j \) uniformly distributed in the range \((-U_0/2, U_0/2)\) and \( \Psi \) the four-orbits basis. Then we can numerically diagonalize the total Hamiltonian and calculate the \( Z_2 \) from the eigenvectors. The result of such a calculation is shown in Fig.(1). Generally all degeneracies except those protected by time-reversal symmetry will be eliminated by disorder. At the TRIM, each eigenvalue of the system is only doubly degenerate. Though the disorder makes the energy spectrum more continuous, a small gap still is clear at half filling. Here the gap location is shifted to the high energy, which is different from the case in the clean system where the gap locates symmetrically at \( E = 0 \). In Fig. 1(a), we start from a topological insulator and introduce weak disorder with the strength \( U_0 = 20 \) meV. It shows in the presence of weak disorder the \( Z_2 \) still has a nontrivial value, which implies that the topological insulator is robust to weak disorder. Instead, in Fig. 1(b), we start from a trivial insulator and introduce strong disorder with the strength \( U_0 = 96 \) meV. The fact of parity product \( \delta = -1 \) at the \( \Gamma \) point and \( \delta = 1 \) at other TRIM for half filling shows that the topological invariant of the system is 1, so the system can obtain non-trivial topological property by introducing strong disorder. We have extended the above calculations to 500 different disorder realizations and the results are stable. So through calculating the \( Z_2 \) invariant, we basically show the effect of disorder in \( HgTe/CdTe \) QWs: the topological phase in the system is not only robust to them, but also can be brought about by introducing them to the trivial phase.

![Figure 1](https://example.com/figure1.png)

**Figure 1.** The eigenvalue and the corresponding parity product at the four TRIM for a \( 24^2 \) super-cell with disorder. Here we start from (a) a topological insulator \( (M = -10 \) meV); (b) a trivial insulator \( (M = 1 \) meV). The red lines in both figures show the gap range which appears at half filling. The other parameters are the same as Ref.[4].

In the presence of disorder, the phase boundary should be determined by the range of the 'mobility' gap. Because there are states in this gap but they are localized, the gap is termed as 'mobility'. The gap from the peaks of the distributions for half filling and the one just above it can be viewed as the 'mobility' gap. This consideration is reasonable in that disorder broadens the energy bands and the broadened part is the most possible one localized by disorder. The phase diagram obtained from the above extracting are shown in Fig.(2). The phase diagram in \( (U_0, E_F) \) plane has also been obtained from conductivity calculations and the SCBA, where the weak-disorder boundary fits well with each other while the strong-disorder boundary does not. Here our result fits well for both the weak- and strong-disorder boundaries, thus the essence of the effect of disorder in the topological phase is obtained. In Fig.2(b), we start from a trivial insulator. As the disorder strength is increased, the system is driven into a topological phase. We study the size effect near the phase transition and find the transition becomes sharper as we increase the lattice size. So it is a direct transition and there is no intermediate phase, which is consistent with the fact of the spin conservation existing in our system. As we further increase the disorder strength, the system firstly is in a stable topological phase and then gradually transitions into a mixed phase, where some fraction of disorder realizations yields a non-trivial topological invariant.
The topological phase with Anderson-type disorder has been discussed by several authors[4, 6]. By calculating the $Z_2$ invariant, we provide some new insights into the phase. In the following, we will consider some other kinds of disorder which may also exist in HgTe/CdTe QWs, such as the fluctuations in the hopping amplitude and the QWs' thickness. There are hopping terms described by the amplitude $D, B, A$ respectively in Hamiltonian Eq.(1). As an example we just introduce disorder to the amplitude $D$ to study the effect of the off-diagonal disorder. It is described by the term $\sum_{j,\delta} U_j \Psi_j^\dagger \Psi_{j+\delta}$ with $j + \delta$ the nearest neighbor site of $j$.

For the disorder in the topological mass, it is described by the term $\sum_j U_j \Psi_j^\dagger (I \otimes \sigma_z) \Psi_j$. In both case, $U_j$ are uniformly distributed in the range $(-U_0/2, U_0/2)$. The results including these two kinds of disorders are shown in Fig.(2). The effect of the disorder in the topological mass is exactly the same as that of the Anderson-type disorder and the phase diagram is consistent with the results from SCBA at weak disorder strengths. While for the case with the disorder in the hopping amplitude, though the effect is similar, the topological phase is destroyed at smaller disorder strength.

**Figure 2.** The phase diagram for the topological phase with disorder in the $(U_0, E_F)$ plane obtained from the super-cell calculations. Still we start from (a) a topological insulator ($M = -10$ meV); (b) a trivial insulator ($M = 1$ meV). The other parameters are the same as those in Fig.1.

4. Conclusions

By calculating the $Z_2$ topological invariant, we study the effects of three kinds of disorders in the nontrivial and trivial phases of HgTe/CdTe QWs. We show that the topological phase in the system is not only robust to these disorders, but also can be brought about by introducing them to the trivial insulator phase. Our these results make a further confirmation and extendability of the study on the interplay between the disorder and the topological phase. At last we mention that the disorder in the hopping amplitude can destroy the topological phase at smaller strengths and a similar theory like SCBA may be developed, which we leave to future work.

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