Kosterlitz–Thouless transition in disordered two-dimensional topological insulators

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Abstract

The disorder-driven metal–insulator transition in the quantum spin Hall systems is studied by scaling analysis of the Thouless conductance \( g \). Below a critical disorder strength, the conductance is independent of the sample size \( M \), an indication of critically delocalized electron states. The calculated beta function \( \beta = \frac{\partial \ln g}{\partial \ln M} \) indicates that the metal–insulator transition is of Kosterlitz–Thouless (KT) type, which is characterized by binding and unbinding of vortex–antivortex pairs of the local currents. The KT-like metal–insulator transition is a basic characteristic of the quantum spin Hall state, being independent of the time-reversal symmetry.

(Some figures may appear in colour only in the online journal)
analysis [20]. Employing a continuum model, Mong et al [21] showed that the surface states of a weak topological insulator with an even number of Dirac cores are delocalized in the absence of a mass term, and localization occurs when the mass term and strong disorder are present. This conclusion may also be applicable to the QSH systems. Xu et al [22] demonstrated numerically that the metallic state in the QSH systems remains robust even when the time-reversal symmetry is broken, in glaring contrast to the trivial unitary class, where all electron states are localized. This result was attributed to the fact that the nontrivial band topology, as described by the spin Chern numbers, is intact when the time-reversal symmetry is broken [17, 23]. The above existing works mainly focus on the issue of whether there exist extended states in the QSH systems, and the answer is affirmative. However, the basic characteristics of the extended states, which determine many of the electron transport properties, have not been carefully investigated. The present work aims to understand these characteristics, and to clarify whether the extended states are strongly delocalized states, as in the usual spin–orbit coupled 2D electron systems, or are critical states, as in the quantum Hall systems.

In this work, from calculations of the Thouless conductance in the Kane–Mele model, it is shown that the disorder-driven metal–insulator transition in the QSH system is a KT phase transition. Below a critical disorder strength, the Thouless conductance \( g \) is found to be independent of the sample size, an indication of critically delocalized electron states. The beta function obtained from the universal scaling function of the conductance vanishes in the metallic phase, with a critical conductivity \( \alpha_c \approx 0.75e^2/h \). Through mapping the local currents onto the local spins in the 2D XY model, we further show that the KT transition is characterized by binding and unbinding of vortex–antivortex pairs. The KT-like metal–insulator transition is a fundamental characteristic of the QSH state, allowing it to be examined experimentally, which neither depends on the time-reversal symmetry, nor requires any long-range correlations of the disorder.

We start from the Kane–Mele model defined on a 2D honeycomb lattice [12, 15, 24], with the Hamiltonian given by

\[
H = -t \sum_{\langle ij \rangle} c_i^\dagger c_j + \frac{2i}{\sqrt{3}} V_{\text{SO}} \sum_i c_i^\dagger \sigma^z (d_i^\dagger \times d_i) c_j + i V_R \sum_i c_i^\dagger \sigma^z (d_i^\dagger \times d_i) c_j + \sum q \epsilon_q c_i^\dagger c_i, \tag{1}
\]

Here, the first term is the usual nearest neighbor hopping term with \( c_i^\dagger = (c_{i\uparrow}^\dagger, c_{i\downarrow}^\dagger) \) as the electron creation operator on site \( i \). The second term is the intrinsic spin–orbit coupling with coupling strength \( V_{\text{SO}} \), where \( \sigma^z \) are the Pauli matrices, \( i \) and \( j \) are two next nearest neighbor sites, \( k \) is their unique common nearest neighbor, and vector \( d_k \) points from \( k \) to \( i \). The third term stands for the Rashba spin–orbit coupling with coupling strength \( V_R \). \( w_i \) is a random on-site energy potential uniformly distributed between \([-W/2, W/2]\), which accounts for nonmagnetic disorder. For convenience, we will set \( \hbar, t \) and the distance between the nearest neighbor sites all to be unity. In the following calculations, \( V_{\text{SO}} = V_R = 0.1 \) is fixed, so the model is inside the QSH phase at \( W = 0 \).

In the following, we follow the standard numerical procedure established in previous works [3–5] to demonstrate the KT nature of the metal–insulator transition. The localization property of an infinite 2D system can be extracted from the scaling analysis of the dimensionless Thouless conductance calculated for finite-size samples [6, 7]. We consider a rectangular sample with two zigzag sides and two armchair sides. Each zigzag side has \( M \) atoms and each armchair side has \( 2M \) atoms, so the sample has a total of \( M \times M \) atoms. The rectangular sample is connected to two semi-infinite leads of the same width with armchair interfaces. At zero temperature, the two-terminal dimensionless Landauer conductance \( g_L \) is calculated from the Landauer–Blüttiker formula [25]

\[
g_L = \frac{\pi}{2} \ln \left| \frac{G_R G_L}{G_L G_L} \right|, \tag{2}
\]

where \( G^{(R)}(E) \) is the retarded (advanced) Green’s function and \( G_L(R)(E) \) is the coupling matrix between the sample and the left (right) lead. The random disorder potential is treated exactly in our finite-size calculations. It is worth mentioning that there exist some other methods to treat the on-site random potential, such as the augmented space techniques [26] or the coherent potential approximation [27]. The Thouless conductance \( g \) is related to the Landauer conductance \( g_L \) through the relation \( 1/g = 1/g_L - 1/N_C \) [5, 28], where \( 1/N_C \) is the contact resistance between the leads and the sample with \( N_C \) as the number of propagating channels in the leads at the Fermi energy \( E \).

Figure 1 shows the size dependence of the calculated conductance \( g \) in logarithmic scale for different disorder strengths
strengths \( W \) at \( E = -1 \) and \(-2\). Periodic boundary conditions are employed in the transverse direction, so that no contribution from edge states is involved. At given values of \( W \) and \( M \), the conductance is averaged over 200–500 random disorder configurations. Symbols with different shapes are used to distinguish data for different \( W \). It is found that the conductance behaves differently with changing sample size in weak and strong disorder regions. For weak disorder, the behavior of \( g \) is unusual in that it neither decreases nor increases with increasing sample size. As a result, the conductance is expected to remain constant in the thermodynamic limit, suggesting that the electron states at the Fermi energy are critically delocalized. For strong disorder, \( g \) decreases with increasing sample size, corresponding to localized states. A metal–insulator transition occurs at an intermediate critical disorder strength.

To further investigate the nature of the metal–insulator phase transition, we perform scaling analysis on the data shown in figure 1 and calculate the beta function \( \beta = d \ln g / d \ln M \). According to the one-parameter scaling theory [6, 7], the localization length in the thermodynamic limit can be extracted by fitting all the data on the insulator side in figure 1 into a universal function \( g = f(M/\xi) \), where the fitting parameter \( \xi \) yields the localization length in the thermodynamic limit. The obtained localization lengths for \( E = -1 \) and \(-2\) are plotted in figures 2(a) and (b), respectively, and the universal scaling function \( g = f(M/\xi) \) is shown in figure 2(c). In the above scaling procedure, only the relative magnitudes of the localization lengths \( \xi \) can be determined. Therefore, we set \( \xi \) at \( W = 6.0 \) to be unity, and the localization lengths for other \( W \) are the relative values with respect to it. It is found that the localization length \( \xi \) as a function of disorder strength \( W \) shown in figures 2(a) and (b) can be fitted with an exponential function \( \xi = e^{\alpha/\sqrt{W - W_C}} \) with \( \alpha \) and \( W_C \) as two fitting parameters. This behavior indicates an exponential decay of the localization length with increasing disorder strength in the insulating phase, which is typical of a KT phase transition [1, 2]. The critical disorder strength for such a metal–insulator transition is obtained as \( W_C = 3.12 \) at \( E = -1 \) and 2.54 at \( E = -2 \), respectively. To facilitate the calculation of the beta function \( \beta = d \ln g / d \ln M \), we fit the data in figure 2(c) with a smooth function, as indicated by the solid line, which is explained below. In the region of small \( \ln(M/\xi) \), the data is fitted with \( g = g_C e^{- (M/\xi)^{1/2}} \), which is consistent with the general behavior of the beta function, \( \beta = 1/ \nu \ln(g/g_C) \), in the quantum critical region \([29]\). On the other hand, a polynomial fit is used in the region of relatively large \( \ln(M/\xi) \). At the boundary between the two regions, \( \ln g \) and its derivative \( \beta \) are required to be continuous.

After obtaining the smooth fitting function describing the scaling relation between \( \ln g \) and \( \ln M \), we take its derivative to calculate the beta function \( \beta = d \ln g / d \ln M \), as plotted in figure 2(d). Here, we note that for weak disorder \((W < W_C)\), where the conductance is nearly independent of the sample size, the localization length diverges and cannot be treated with the same scaling procedure as above. Instead, we fit the logarithmic conductance \( \ln g \) as a function of \( \ln M \) with straight lines, and take their slopes as the values of \( \beta \), which are shown by the diamonds in figure 2(d). We see from figure 2(d) that \( \beta \) increases with
that a minimum (critical) conductivity, $\sigma_c$ systems [3–5]. The behavior of the beta function also suggests that the disorder-driven metal–insulator transition is a KT transition, as observed in other disordered 2D electron systems [3–5]. The behavior of the beta function also suggests that a minimum (critical) conductivity, $\sigma_c = g_c(e^2/h)/\sqrt{3} \approx 0.75(e^2/h)$ (1/$\sqrt{3}$ being the aspect ratio), exists for the bulk QSH system.

An important characteristic of the traditional KT transition in the $XY$ model is the binding of vortex–antivortex pairs in the ordered phase near the transition point and unbinding in the disordered phase [1, 2]. For 2D electron systems, Zhang et al [5] proposed to map the local currents onto the local spins in the $XY$ model. The bond current vector between sites $m$ and $n$ can be calculated by [5, 30, 31]

$$i_{m \rightarrow n} = \frac{-2e}{h} \int \frac{dE}{2\pi} \text{Re}[H_{m \rightarrow n} G_{m \rightarrow n}(E)],$$

where $\sigma_1$ and $\sigma_2$ represent the spin index and $G_{m \rightarrow n}(E)$ is the matrix element of the lesser Green’s function. The lesser Green’s function is given by

$$G^<(E) = G^>(E) \left[ i \sum_n \Gamma_n(E) f_0(E) \right] G^>(E),$$

where $f_0(E) = f_0(E + eV_o)$ is the Fermi distribution function in lead $\alpha$ with $V_o$ as the electrical potential in the lead. The local current vector defined on site $n$ is $i_n = \sum_{m \rightarrow n} i_{m \rightarrow n}$ [5], where the vectorial summation is taken over all the nearest and next nearest neighbors $m$ of site $n$. Along a closed path, the polar angle $\theta_n$ of $i_n$ is considered to change continuously with changing coordinates, and a topological charge is defined as $c = \frac{1}{2\pi} \oint \nabla \cdot dl$, where the path integral is counterclockwise [5]. A nonzero number of $c$ indicates the appearance of a vertex ($c > 0$) or an antivortex ($c < 0$). Figure 3 shows typical distributions of the topological charges on the two sides of the metal–insulator transition. The arrows in the figure indicate only the direction of the local currents, without showing the magnitude for the purpose of visualization. In the delocalized phase (figure 3(a)), a few vortices ($c > 0$) and antivortices ($c < 0$) are excited in pairs and bounded together, corresponding to the ordered phase at low temperature in the 2D $XY$ model. In the localized phase (figure 3(b)), a large number of vortices and antivortices appear and are mostly unbounded, corresponding to the disordered phase at high temperature.

Finally, we study the effect of breaking the time-reversal symmetry on the KT phase transition, by including a new term $\vec{h} \cdot \vec{\sigma}$ into Hamiltonian (1), where $\vec{h}$ stands for a uniform Zeeman field. The calculated conductances at $E = -1$ and $-2$ as functions of sample size $M$ for different disorder strengths are shown in figures 4(a) and (b) for a vertical Zeeman field $\vec{h} = (0, 0, h_z = 0.1)$ and in figures 4(c) and (d) for a horizontal field $\vec{h} = (h_x = 0.1, 0, 0)$. The parameters are chosen in such a manner that the system is in the time-reversal symmetry broken QSH phase in the clean limit [22, 23]. The conductance shown in figures 4(a)–(d) displays similar size dependence to that in figure 1. For weak disorder, the conductance is nearly independent of sample size, indicating the existence of the critically delocalized states. For strong disorder, the conductance decreases with sample size, indicating that the electron states are localized. It is found that all the data on the insulating side in figures 4(a)–(d) can also be fitted with a universal scaling function $g = f(M/\xi)$, as shown in figure 4(e). In figure 4(f), the beta function (solid line) for the time-reversal symmetry broken QSH system is obtained in the same way as in figure 2. As expected, the beta function vanishes above a critical
Figure 4. (a)–(d) Conductance as a function of sample size with Fermi energy $E$, in the presence of a vertical Zeeman field $h_z$ or a horizontal Zeeman field $h_x$. (e) Universal scaling function $g = f(M/\xi)$, where the solid line represents a smooth functional fit to the data. (f) The corresponding beta functions for the time-reversal symmetry broken QSH system (solid line) and time-reversal symmetry invariant QSH system (dotted line).

In summary, the metal–insulator transition in the QSH systems is studied based upon the scaling analysis of the Thouless conductance. The disorder-driven metal–insulator transition is found to be a KT-like transition, characterized by binding and unbinding of vortex–antivortex pairs of local electrical currents. The beta functions for the QSH systems with and without the time-reversal symmetry are close to each other on the metallic side, but somewhat different on the insulating side, the latter being attributed to the fact that they belong to different symmetry classes. Our work has established a fundamental property of the QSH state, which can be observed experimentally. Study of the electron–electron interaction effect, which is expected to favor the metallic behavior and increase the beta function in the metallic phase, will be left to future works.

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