Delocalization of Surface Dirac Electrons in Disordered Weak Topological Insulators

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The spectrum of massless Dirac electrons on the side surface of a three-dimensional weak topological insulator is significantly affected by whether the number of unit atomic layers constituting the sample is even or odd; it has a finite-size energy gap in the even case while it is gapless in the odd case. The conductivity of such a two-dimensional Dirac electron system with quenched disorder is calculated when the Fermi level is located at the Dirac point. It is shown that the conductivity increases with increasing disorder and shows no clear even-odd difference when the aspect ratio of the system is appropriately fixed. From the system-size dependence of the average conductivity, the scaling function \( \beta \) is determined under the one-parameter scaling hypothesis. The result implies that \( \beta = 0 \) in the clean limit at which the conductivity is minimized, and that \( \beta > 0 \) otherwise. Hence, the system is a perfect metal in the thermodynamic limit except in the clean limit that should be regarded as an unstable fixed point.

Three-dimensional topological insulators are characterized by four \( \mathbb{Z}_2 \) indices, the strong index \( \nu_0 \) and the weak indices \( \nu_1, \nu_2, \) and \( \nu_3 \).\(^{1–3} \) The strong index distinguishes a strong topological insulator (STI) with \( \nu_0 = 1 \) from a weak topological insulator (WTI) and a trivial insulator with \( \nu_0 = 0 \). Among the sectors of \( \nu_0 = 0 \), a WTI is characterized by the condition that at least one of the weak indices is nonzero. The most notable feature of STI and WTI is that low-energy electron states described by a massless Dirac equation appear on their surfaces. They are called Dirac electrons and possess a linear energy dispersion forming a gapless conic structure (i.e., Dirac cone) in the reciprocal space. A crucial difference between STI and WTI is that Dirac electrons have different symmetries without the spin-rotation invariance.\(^{4–13} \) Several materials have been proposed as candidates for a WTI.\(^{14–17} \)

Dirac electrons on the side surface of a WTI show unusual properties that depend on the number of unit atomic layers stacked along \( \mathbf{v} \) is even or odd.\(^{6,9,10} \) Note that the unit atomic layer can be regarded as a two-dimensional (2D) quantum spin Hall insulator possessing a one-dimensional helical edge channel.\(^{1} \) A series of helical edge channels forms a Dirac electron system on the side surface. If the number of unit atomic layers is even, the helical edge channels acquire a finite-size gap as a result of their mutual coupling. Contrastingly, in the odd case, one helical channel survives without being gapped out. Another important property arises from the fact that regardless of the location of the Fermi level, the number of conducting channels is even in the even case and odd in the odd case. This parity leads to a notable difference in the transport property of disordered systems. From a symmetry viewpoint, Dirac electrons have symplectic symmetry that preserves the time-reversal symmetry without the spin-rotation invariance.\(^{18} \) It has been shown that a disordered system with symplectic symmetry has a perfectly conducting channel in the odd-channel case,\(^{19} \) and that this crucially affects the transport property in a quantum wire structure;\(^{20–24} \) the system with even channels becomes insulating in the long-wire limit while that with odd channels remains metallic. This observation holds for the Dirac system on the side surface of a WTI.\(^{6} \)

Let us consider a 2D Dirac electron system on the surface of WTI systems, focusing on its transport properties in the large area limit. An important question is whether it is localized by quenched disorder.\(^{6} \) In the case of an STI, it has been demonstrated that the 2D Dirac system with one Dirac cone is a perfect metal.\(^{25,26} \) The case of a WTI with two Dirac cones has been studied by Mong et al.\(^{7} \) and Obuse et al.\(^{13} \) using a finite-size scaling approach.\(^{27} \) Both of them conclude that the system is again a perfect metal showing no sign of Anderson localization. However, there remain subtle issues to resolve. Mong et al. derived a scaling relation of the conductivity on the ba-
sis of a microscopic model consisting of two Dirac cones. This model is plausible but involves no even-odd feature since it is defined on a 2D continuous space. Obuse et al. elaborately studied the localization problem by using a network model\cite{13,28} in which the presence of a perfectly conducting channel is encoded. However, they did not explicitly present a scaling relation of the conductivity including its parity dependence.

In this letter, we numerically study the localization problem on the surface of a WTI using a microscopic model that correctly describes the even-odd difference. Our attention is focused on the case of the Fermi level being located at the Dirac point\cite{25} since the conductivity is expected to be minimized there.\cite{29,30}

We numerically calculate the average conductivity of disordered systems of length $L$ and width $W$ at a fixed ratio $R = L/W$, and analyze its behavior using a finite-size scaling approach. We separately treat the even and odd cases. It is shown that the $L$ dependence of the average conductivity becomes parity-independent if $R$ is sufficiently small. It is also shown that the average conductivity increases with increasing disorder and is minimized in the clean limit. From the numerical result, we determine the scaling function $\beta$ under the one-parameter scaling hypothesis.\cite{27}

The result implies that $\beta > 0$ except in the clean limit that should be regarded as an unstable fixed point of $\beta = 0$. That is, the system becomes a perfect metal with increasing system size, except at the unstable fixed point. We set $\hbar = 1$ throughout this letter.

We consider the side surface of width $W$ on the $xy$-plane being infinitely long in the $z$-direction. It consists of $M$ unit atomic layers stacked in the $y$-direction and the width is $W = Ma$ with $a$ being the lattice constant. Each unit layer has one helical edge channel aligned with the $x$-axis, and the resulting $M$ helical channels form the 2D Dirac system by coupling with their nearest neighbors. The region of $L \geq x \geq 0$ is regarded as the sample with disorder, and the region of $x < 0$ ($x > L$) plays a role of the left (right) lead. Let $\{j\} \equiv \{j\uparrow, j\downarrow\}$ be the two-component vector representing the state in the $j$th helical channel ($M \geq j \geq 1$), where $\uparrow$ and $\downarrow$ specify the spin direction. It is assumed below that the up-spin (down-spin) state propagates in the right (left) direction. We adopt the following effective Hamiltonian for the surface state of a WTI.\cite{12,13}

$$
H_{\text{eff}} = \sum_{j=1}^{M} \langle j | \begin{pmatrix} -iv\partial_x + U(x) & 0 \\ 0 & iv\partial_x + U(x) \end{pmatrix} | j \rangle + \sum_{j=1}^{M-1} \left\{ \begin{array}{l} \langle j + 1 | \begin{pmatrix} 0 & \frac{\sigma_y}{2a} \\ -\frac{\sigma_y}{2a} & 0 \end{pmatrix} | j \rangle + \text{h.c.} \end{array} \right\}.
$$

(1)

The potential $U(x)$ is included to simulate the setup\cite{31} in which the Fermi level is fixed at the Dirac point ($\epsilon = 0$) in the sample region, while the right and left leads are deeply doped. That is, we set $U(x) = 0$ in the sample region, and $U(x) = -U_0$ outside the sample with $U_0$ being positive and large.

Let us briefly describe the wave functions at an energy $\epsilon$ in the case of $U(x) \equiv 0$. Our model has two Dirac cones centered at $(0, 0)$ and $(0, \pi/a)$ in the reciprocal space. The transverse function is constructed by superposing two wave functions of different Dirac cones as \cite{9}

$$
\chi_m(j) = c_m \left( e^{iq_m y_j} - (-1)^j e^{-iq_m y_j} \right)
$$

(2)

with $y_j \equiv ja$, where $c_m$ is the normalization constant and $q_m = m\pi/[(M+1)a]$ with

$$
m = \frac{M+1}{2}, \frac{M+3}{2}, \ldots, -\frac{M-1}{2}.
$$

(3)

The subband energy of the $m$th mode is $\Delta_m = (v/a)\sin q_m a$, and the dispersion relation as a function of the longitudinal wave number $k \equiv \epsilon_m(k) = \pm \sqrt{(vk)^2 + \Delta_m^2}$. For an odd $M$, we see that $\Delta_m$ vanishes for $m = 0$, indicating that the system has gapless excitations. For an even $M$, $m = 0$ is not allowed so a finite-size gap opens across the Dirac point (see Fig. 1). If $|\epsilon| > \Delta_m$, the $m$th mode provides two counterpropagating channels. The corresponding wave functions $\varphi_m^\pm(x, j)$ are

$$
\varphi_m^\pm(x, j) = \frac{1}{\sqrt{\epsilon_m}} \chi_m(j) e^{\pm ik_m x} \begin{pmatrix} a_m^\pm \\ b_m^\pm \end{pmatrix},
$$

(4)

where $\pm$ specifies the propagating direction, $k_m = \sqrt{\epsilon^2 - \Delta_m^2}/v$, and

$$
\begin{pmatrix} a_m^\pm \\ b_m^\pm \end{pmatrix} = \frac{1}{\sqrt{\epsilon^2 + (\pm vk_m - \Delta_m)^2}} \begin{pmatrix} i\eta_m \Delta_m \pm vk_m - \epsilon \\ \pm \Delta_m \nu_{k_m} \end{pmatrix},
$$

(5)

where $\eta_m = 1$ for $m > 0$ and $-1$ for $m < 0$. The group velocity $v_m$ is obtained as $v_m = v(\nu_{k_m}/|\epsilon|)$. In the case of $|\epsilon| < \Delta_m$, the $m$th mode provides two evanescent channels. The corresponding wave functions are obtained from Eq. (4) by the following replacement: $k_m \rightarrow i\kappa_m$ with $\kappa_m = \sqrt{\Delta_m^2 - \epsilon^2}/v$. The group velocity has no physical meaning for evanescent channels.

To incorporate disorder, we add the potential $V$ consisting of $\delta$-function-type impurities in the sample region,
let us briefly consider the conductivity of propagating parts. Once they are evaluated, we can construct the transmission matrix for a given impurity configuration is obtained as \[ \sigma_{\text{cl}} = \sum_{m} \cosh^{-2}(\Delta_{m} L/v). \] Note that the term with \( m = 0 \) for an odd \( M \) corresponds to a perfectly conducting channel. In Fig. 2, \( \sigma_{\text{cl}} = (L/W)g_{\text{cl}} \) at \( L/a = 1000 \) is plotted for the even and odd cases as a function of the aspect ratio \( R = L/W \). We see from Fig. 2 that \( \sigma_{\text{cl}} \) shows no even-odd difference if \( R \) is sufficiently small. This suggests that the case of \( R \ll 1 \) is suitable for capturing a parity-independent scaling flow, while computations for a given \( L \) become heavier with decreasing \( R \). Considering these two points, we set \( R = 1/3 \) hereafter. Note that \( \sigma_{\text{cl}}(L) \) is a monotonically decreasing function of \( L \) and converges in the large-\( L \) limit. At \( R = 1/3 \), we find that \( \sigma_{\text{cl}}(\infty) \approx 0.6386 \) in the odd-\( M \) case and \( \sigma_{\text{cl}}(\infty) \approx 0.6347 \) in the even-\( M \) case. If \( R \ll 1 \), \( \sigma_{\text{cl}}(\infty) = 2/\pi \approx 0.6366 \) with no parity dependence. We show below that \( \sigma_{\text{cl}} \) is the lower limit of the average conductivity.

Now, we present the numerical result for the average conductivity \( \langle \sigma \rangle \). The system size is varied from \( M \times N = 30 \times 10 \) to \( 270 \times 90 \) in the even-\( M \) case and from \( 33 \times 11 \) to \( 303 \times 101 \) in the odd-\( M \) case, where the aspect ratio is fixed at \( R = 1/3 \). The number of impurities is also fixed as \( N_{\text{imp}} = M \times N \), resulting in \( \Gamma = (a/v)^2 V_{0}^2 \). The strength of disorder is tuned as \( \Gamma = 0.2 - 8.0 \) by adjusting \( V_{0} \). In performing the ensemble average, the number of samples, \( N_{\text{sam}} \), is set to 5000 for each data point. The \( L \)-dependence of \( \langle \sigma \rangle \) is shown in Fig. 3(a), where open (filled) symbols correspond to the odd-\( M \) (even-\( M \)) case, and the dashed (solid) line represents \( \sigma_{\text{cl}}(L) \) in the odd-\( M \) (even-\( M \)) case. The strength of disorder is \( \Gamma = 0.2, 0.4, 0.5, 0.6, 0.8, 1.0, 1.2, 1.5, \) and 2.0 from bottom to top. If the numerical uncertainty \( \Delta \sigma \) is defined by \( \Delta \sigma = \langle \text{var} \rangle / N_{\text{sam}}^{1/2} \) following Ref. 32, the relative uncertainty \( \Delta \sigma / \langle \sigma \rangle \) is smaller than 0.003 at each data point. No clear even-odd difference appears in Fig. 3(a). We see that \( \langle \sigma \rangle \) increases with increasing \( \Gamma \), indicating that \( \langle \sigma \rangle \) is minimized in the clean limit, i.e., \( \langle \sigma(L) \rangle \geq \sigma_{\text{cl}}(L) \). Although \( \langle \sigma \rangle \) slightly decreases with increasing \( L \) at a small \( \langle \sigma \rangle \), this should not be regarded as a sign of localization. Note that \( \langle \sigma(L) \rangle \) at \( \Gamma = 0.2 \) (the lowest data set) is very close to \( \sigma_{\text{cl}}(L) \) represented by the solid and dashed lines. This indicates that the decreasing behavior is induced by a finite-size correction reflecting a weak \( L \)-dependence of \( \sigma_{\text{cl}} \). To reduce it, we introduce the renormalized conductivity \( \langle \sigma(L) \rangle \) defined by \( \langle \sigma(L) \rangle = \langle \sigma(L) \rangle - \delta \sigma_{\text{cl}}(L) \), where the finite-size correction \( \delta \sigma_{\text{cl}}(L) \equiv \sigma_{\text{cl}}(L) - \sigma_{\text{cl}}(\infty) \) is a monotonically decreasing function of \( L \). We treat \( \langle \sigma(L) \rangle \) instead of \( \langle \sigma(L) \rangle \) in the following analysis.
The $L$ dependence of $\langle \langle \sigma \rangle \rangle$ is shown in Fig. 3(b). We see that $\langle \langle \sigma \rangle \rangle$ clearly increases with increasing $L$. An exception is the case of $\Gamma = 0.2$ (the lowest data set), where $\langle \langle \sigma \rangle \rangle$ seems almost independent of $L$. However, this does not deny a plausible hypothesis that $\langle \langle \sigma \rangle \rangle$ increases very slowly with increasing $L$ even when $\Gamma$ is small. We demonstrate in Fig. 4 that the data sets for $\Gamma = 0.3$–8.0 collapse onto one scaling curve by shifting the data horizontally. Here, only the data in the odd-$M$ case are plotted in Fig. 4. We see that the scaling curve is approximated as

$$\langle \langle \sigma \rangle \rangle = \text{const.} + \frac{1}{8} \ln(L/a^*)$$

at a large $\langle \langle \sigma \rangle \rangle$, indicating the presence of the weak antilocalization correction. We also see that the renormalized conductivity decreases toward a limiting value, $\sigma^*$, with decreasing $L/a^*$. Although $\sigma^*$ cannot be precisely determined from our data, it is bounded from below by the clean-limit value $\sigma_{cl}(\infty)$. We adopt the most plausible conjecture that $\sigma^* = \sigma_{cl}(\infty)$ since there is no reason to believe that $\sigma^*$ is larger than $\sigma_{cl}(\infty)$. The scaling function $\beta$, defined by

$$\beta(\langle \langle \sigma \rangle \rangle) = \frac{d\ln(\langle \langle \sigma \rangle \rangle)}{d\ln L},$$

is shown in Fig. 5. Equation (12) indicates that $\beta$ at a large $\langle \langle \sigma \rangle \rangle$ is expressed as $\beta = (1/8)\langle \langle \sigma \rangle \rangle^{-1} > 0$. In the opposite regime of $\langle \langle \sigma \rangle \rangle$ being close to $\sigma_{cl}(\infty)$, we expect that $\beta$ decreases with decreasing $\langle \langle \sigma \rangle \rangle$ and finally vanishes at $\sigma_{cl}(\infty)$. Thus, $\beta$ is always positive except at $\sigma_{cl}(\infty)$. This is in marked contrast to the case of ordinary 2D systems with symplectic symmetry, where $\beta$ becomes negative when the conductivity falls below a critical value.

Here, let us briefly consider the case of $R$ being greater than $1/3$. In this case, since the clean-limit conductivity $\sigma_{cl}(\infty)$ depends on the even-odd parity as well as on $R$, we expect that the scaling function at a small $\langle \langle \sigma \rangle \rangle$ will split into two curves corresponding to the even and odd cases. We also expect that the two curves will merge at a large $\langle \langle \sigma \rangle \rangle$ since the weak antilocalization correction should be insensitive to the parity.

The above argument indicates that the conductivity of the system monotonically increases with increasing system size, except at an unstable fixed point corresponding to the clean limit. It is conceivable that such an unstable fixed point also exists in 2D massless Dirac electron systems with one Dirac cone.

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