Effect of surface disorder on the chiral surface states of a three-dimensional quantum Hall system

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We investigate the effect of surface disorder on the chiral surface states of a three-dimensional quantum Hall system. Utilizing a transfer matrix method, we find that the localization length of the surface state along the magnetic field decreases with the disorder strength in the weak disorder regime, but increases anomalously in the strong disorder regime. In the strong disorder regime, the surface states mainly locate at the first inward layer to avoid the strong disorder in the outmost layer. The anomalous increase of the localization length can be explained by an effective model, which maps the strong disorder on the surface layer to the weak disorder on the first inward layer. Our work demonstrates that surface disorder can be an effective way to control the transport behavior of the surface states along the magnetic field. We also investigate the effect of surface disorder on the full distribution of conductances $P(g)$ of the surface states in the quasi-one-dimensional (1D) regime. In particular, we find that $P(g)$ is Gaussian in the quasi-1D metal regime and log-normal in the quasi-1D insulator regime. In the crossover regime, $P(g)$ exhibits highly nontrivial forms, whose shapes coincide with the results obtained from the Dorofohov-Mello-Pereyra-Kumar equation of a bulk-disordered quasi-1D wire in the absence of time-reversal symmetry. Our results suggest that $P(g)$ is fully determined by the average conductance, independent of details of the system, in agreement with the single-parameter scaling hypothesis.

I. INTRODUCTION

The quantum Hall effect (QHE) in two-dimensional (2D) electron systems originates from discrete Landau levels forming under a strong perpendicular magnetic field. In three-dimensional (3D) systems, the band dispersion along the magnetic field (z axis) usually closes the quantum Hall gap. However, if the interlayer coupling is small compared to Landau level spacing, we expect the QHE still exists. This idea was realized in an engineered multilayer quantum well system, and very recently, in an anisotropic layered material BaMnSb. Even if the interlayer coupling is large enough to close the quantum Hall gap, a gap may further be induced by spontaneous charge density wave in the z direction under a strong magnetic field. The 3D QHE recently observed in ZrTe$_2$ and HfTe$_2$ are suggested to be this type. Signatures of 3D QHE have also been found in Bechgaard salt, $\kappa$-Mo$_2$O$_3$, graphene, $n$-doped Bi$_2$Se$_3$, and EuMnBi$_2$. These materials offer us great opportunities to study the QHE beyond two dimensions.

The distinct feature of a 2D quantum Hall system is its chiral edge states, which are topologically protected by the bulk gap and robust against disorder. In the 3D case, the chiral edge state of each layer is coupled to neighboring edge states, forming a 2D chiral surface state. The transport properties of this chiral surface states turn out to be highly anisotropic in the presence of disorder. Due to the chiral nature of the surface states, the in-plane transport is ballistic. In the vertical direction, interestingly, there exist three distinct regimes in a mesoscopic sample, namely, 2D chiral metal, quasi-one-dimensional (1D) metal, and quasi-1D insulator.

The existence of the 2D chiral surface states was confirmed in Refs. The so far, however, the three transport regimes of the surface states have not been investigated in experiments.
der strength increases, the localization length decreases in the weak disorder regime but increases anomalously in the strong disorder regime. The main weight of the surface state gradually moves from the outmost layer to the first inward layer, and finally forms a weakly disordered surface state beneath the disordered surface layer in the large disorder limit. The anomalous increase of the localization length in the strong disorder regime can be explained by an effective model, which maps the strong disorder on the surface to the weak disorder on the first inward layer. Our results demonstrate that surface disorder can be an effective way to control the transport behavior of the surface states in the z direction. For the localized surface state in the intermediate disorder regime, the conduction can be further enhanced by doping disorder on its surface, forming a more extended state beneath the outmost disordered layer.

We also investigate the effect of surface disorder on the conductance distributions \( P(g) \) of the chiral surface states in the quasi-1D regime. Numerical investigations of \( P(g) \) of the chiral surface states are rather limited in the literature. To the best of our knowledge, the only work was done in Ref.\(^{[23]} \), which studied \( P(g) \) using the 2D directed network model in the quasi-1D regime. In the presence of strong surface disorder, the 2D directed network model is no longer valid.\(^{[24,44,45]} \) Using the 3D tight-binding model, we find that \( P(g) \) is Gaussian in the quasi-1D metal regime and log-normal in the quasi-1D insulator regime as expected. In the crossover regime, \( P(g) \) is found to exhibit highly nontrivial forms, whose shapes coincide with the results obtained from the Dorokhov-Mello-Pereyra-Kumar (DMPK) equation of a bulk-disordered quasi-1D wire in the absence of time-reversal symmetry (unitary universality class.\(^{[22,44,45]} \)) Our results suggest that \( P(g) \) is the only function of the average conductance, independent of the surface disorder strength and the size of the system, in agreement with the single-parameter scaling hypothesis.

The rest of the paper is organized as follows. In Sec.\(^{[2]} \) we describe the tight-binding Hamiltonian for 3D quantum Hall system and the numerical method we use. In Sec.\(^{[3]} \) we present our numerical results. The paper is summarized in Sec.\(^{[5]} \).

\section{Model and Method}

We consider an electron on an \( L_x \times L_y \times L_z \) cubic lattice in the presence of a magnetic field \( B \hat{z} \) with tight-binding Hamiltonian

\[
\mathcal{H} = - \sum_{\langle \mathbf{i}, \mathbf{j} \rangle} \left( t_{ij} e^{i \theta_{ij}} c_{i}^{\dagger} c_{j} + h.c. \right),
\]

where we have anisotropic nearest-neighboring hopping

\[
t_{ij} = \begin{cases} 
1 & \text{if } i \text{ and } j \text{ are horizontal nearest neighbors,} \\
2 & \text{if } i \text{ and } j \text{ are vertical nearest neighbors,} \\
0 & \text{if } i \text{ and } j \text{ are not nearest neighbors.}
\end{cases}
\]

We choose Landau gauge \( \hat{A} = (0, Bx, 0) \) and define \( \theta_{ij} = \frac{\xi}{\hbar} \int_{l}^{j} \hat{A} \cdot d\mathbf{l} \). The magnetic flux \( \phi \) per unit cell in a horizontal plane is

\[
\frac{\phi}{\phi_0} = \frac{B a^2}{\hbar c/e} = \frac{1}{2\pi} \sum_{\square} \theta_{ij},
\]

where \( \phi_0 = \hbar c/e \) is the flux quantum.

In the 2D limit with \( L_z = 1 \), this model has a butterfly-like self-similar energy spectrum, as the flux \( \phi \) per unit cell varies.\(^{[26]} \) When the flux \( \phi \) per unit cell is chosen as \( \phi_0/N \) for integer \( N \), there are exactly \( N \) subbands in the spectrum. Here, we consider the case where \( t_z \) is much smaller than the horizontal hopping \( t_1 = 1 \), so that the subband gaps are not closed by the dispersion in \( z \) axis. The 2D chiral surface states lie in the gap regions between the subbands and can be revealed by imposing open boundary conditions in the \( x \) and \( y \) directions.

To study the effect of surface disorder on the surface states, we consider the random on-site potential given by

\[
\mathcal{H}_{\text{imp}} = \sum_{i} \epsilon_i c_i^{\dagger} c_i,
\]

where \( \epsilon_i \) are independent variables with identical uniform distribution on \([−W/2, W/2]\). The effect of bulk disorder on this system has been studied in Refs.\(^{[35,36]} \). Here we consider surface disorder and introduce disorder only for the sites at the outmost sidewalls of the sample.

To calculate the two-terminal conductance, we attach two semi-infinite clean leads at the top and bottom ends of the sample. The conductance is calculated from the Landauer-Büttiker formula\(^{[37]} \)

\[
G = \frac{2e^2}{h} \text{Tr}(t t^\dagger).
\]

In it, \( t \) is the transmission matrix, which we calculate using the transfer matrix method\(^{[46,48]} \). For simplicity, we use the dimensionless conductance \( g \) defined as \( g = G/(2e^2/h) \) in the rest of the paper.

\section{Results}

\subsection{Localization length}

Due to the chiral nature of the edge states, the transport of the surface states is ballistic in the \( x \)-\( y \) plane. Furthermore, the unidirectional transport in the \( x \)-\( y \) plane suppresses the localization effect in the \( z \) direction. In order to make quantum interference happen, an electron has to circumnavigate the sample and return to its starting point. This is impossible in an infinite sample. Thus, for an infinite sample, vertical transport is always diffusive, independent of the disorder strength.\(^{[22]} \)

In a mesoscopic sample, an electron can circle the sample and interfere with itself. For very long length \( L_z \), the system is of quasi-1D nature. The interference can happen many times so that the surface state is localized in the \( z \) direction. This is the so-called quasi-1D insulator regime of the chiral surface states. For \( l \ll L_z \ll \xi \), where \( l \) is the mean free path and \( \xi \) is
the localization length, the system is in the diffusive regime. Here another characteristic length scale emerges and separates the diffusive regime into two regimes. During one round-trip of the sample, an electron diffuses a distance $L_0$ in the vertical direction. If $L_0 \ll L_z \ll \xi$, that means the electron circles around the sample many times before diffusing out, the system is in the quasi-1D metal regime. If $l \ll L_z \ll L_0$, the electron diffuses out of the sample without a complete round-trip, the system is in the 2D chiral metal regime. In terms of the average conductance, both regimes share the same Ohmic behavior. However, the conductance fluctuations can be much larger in the 2D chiral metal regime, since the system can be effectively broken up into independent parallel strips, whose width is the distance an electron propagates in the chiral direction during the trip. We note that to avoid entering into the ballistic regime, the system size needed for the 2D chiral metal regime is rather large for a 3D tight-binding Hamiltonian. Therefore, we focus on the quasi-1D metal and insulator regimes in this paper.

The characteristic length scale that separates the quasi-1D metal and insulator regimes is the localization length $\xi$. First, we study how the surface disorder strength affects the localization length of the surface states in the $z$ direction. The localization length can be determined from the scaling behavior of the average conductance. For relatively short samples, the average conductance follows a typical Ohmic behavior. For relatively long samples, the average conductance decays exponentially with the length $L_z$ in the form

$$\langle \ln g \rangle \sim -\frac{2L_z}{\xi}. \quad (5)$$

The crossover from the quasi-1D metal to insulator regime occurs at $\langle \ln g \rangle \sim 1$, where $L_z$ is of the order of $\xi$. Figure 1 shows $\langle \ln g \rangle$ as a function of $L_z$ in a quasi-1D system $L \times L \times L_z$ for two different transverse system sizes $L = 21$ and 30. Here, we choose $\phi = \phi_0/3, \tau_z = 0.1$, and $W = 1$. The energy is at $E = -1.35$, which is near the center of the subband gap. We obtain the localization lengths from the linear parts of the curves by using Eq. (5). The fitting yields $\xi = 49.2 \pm 2.3$ for $L = 21$ and $\xi = 65.3 \pm 2.1$ for $L = 30$. For a quasi-1D system, the localization length is expected to be proportional to the number of conducting channels $N$. Since the number of conducting channels of the surface states is proportional to the circumference of the sample, the localization length is approximately proportional to the width $L$ in our case.

By repeating the above procedure, we calculate the localization length as a function of the disorder strength in Fig. 2. For both widths $L$, the localization length decreases as the disorder strength increases at weak disorder. However, after a critical disorder strength $W_c$, which is of the order of the bandwidth, the localization length increases anomalously with the disorder strength. In other words, the conduction of the surface state is enhanced by surface disorder in this regime.

To understand the anomalous increase of the localization length in the strong disorder regime, in Fig. 3 we plot the typical surface states in a $21 \times 21 \times 21$ cubic lattice at $E = -1.35$ for $W = 1, 6, 150$. For weak disorder $W = 1$, the surface state mainly locates at the outermost layer and is extended in the $z$ direction. At intermediate disorder $W = 6$, the surface state moves inward significantly, it becomes inhomogeneous in the $x-y$ plane and localized in the $z$ direction. For very strong disorder $W = 150$, the surface state mainly locates at the first inward layer and becomes extended again in the $z$ direction. The surface states in the $x-y$ plane are topologically protected by the bulk gap of the system. Since surface disorder does not alter the bulk gap, it never destroys the surface states in the $x-y$ plane. For very strong disorder, the surface layer becomes an Anderson insulator. The redistributed surface state on the first inward layer can be considered as an interface state between an Anderson insulator and a 3D quantum.
FIG. 4. The probability $P(d) = \int d^3\vec{x} |\psi(\vec{x})|^2 \delta(d - d(\vec{x}))$ as a function of distance $d$ from the surface in a $21 \times 21 \times 21$ cubic lattice at $E = -1.35$ for $W = 0, 6, 11, 40, \text{ and } 150$. Here $\phi = \phi_0/3$, $t_z = 0.1$. The average is taken over $10^3$ disorder realizations. As the disorder strength increases, the main weight of the surface state gradually moves from the outmost layer to the first inward layer.

Schrödinger equation of the whole system can be written as

$$\begin{pmatrix} H_0 & V \\ V^\dagger & H_{\text{dis}} \end{pmatrix} \begin{pmatrix} \psi_0 \\ \psi_{\text{dis}} \end{pmatrix} = E \begin{pmatrix} \psi_0 \\ \psi_{\text{dis}} \end{pmatrix},$$

(6)

where $H_0$ is the Hamiltonian for the clean bulk, $H_{\text{dis}}$ is the Hamiltonian for the disordered surface layer, $V$ and $V^\dagger$ are the couplings between them, and $\psi_0$ and $\psi_{\text{dis}}$ are the corresponding wave functions. In the strong disorder regime, $W \gg t$, $\psi_{\text{dis}}$ may be considered as a high-energy sector and can be integrated out. Eliminating $\psi_{\text{dis}}$ in Eq. (6), we obtain an effective Hamiltonian for the clean bulk

$$H_0 - \frac{VV^\dagger}{H_{\text{dis}} - E} \psi_0 = E\psi_0,$$

(7)

which means the disorder potential on the first inward layer is renormalized into $V(H_{\text{dis}} - E)^{-1}V^\dagger$. Physically, this term describes the virtual hopping from the clean bulk to the high-energy states on the disordered surface layer, and finally back to the bulk. Since the matrix elements of $V$ are of the order of $t$, the effective disorder on the first inward layer is of the order $t^2/W$, which is much weaker than the disorder strength $W$ on the outmost layer. As $W$ increases, the effective disorder on the first inward layer decreases. This explains the anomalous increase of the localization length in the strong disorder regime.

B. Conductance distributions

So far, we have investigated the effect of surface disorder on the localization length of the chiral surface states in the $z$ direction, which can be determined from the scaling of the average conductance. In the following, we consider the effect of surface disorder on the full distribution of the conductances in the quasi-1D regime.
The conductance distributions of the chiral surface states have been mainly investigated using a 2D directed network model in the literature. In Ref. [23], Gruzberg, Read, and Sachdev proved that in the quasi-1D regime, the conductance properties of the 2D directed network model are the same as that of a bulk-disordered quasi-1D wire. The latter has been extensively investigated, and a nearly complete description of the conductance properties is available in the literature [52,53].

The first two moments of the conductance distribution have been calculated for all disorder strength using the supersymmetric nonlinear $\sigma$ model [53]. Furthermore, the full probability distribution of the transmission eigenvalues $P(T_n)$ can be obtained from the DMPK equation of the Fokker-Planck approach [54]. The DMPK equation describes the evolution of $P(\{\lambda_n\})$ with increasing wire length $L_z$ [50].

$$i \frac{\partial P}{\partial L_z} = \frac{2}{\beta N + 2 - \beta} \sum_{n=1}^{N} \frac{\partial}{\partial \lambda_n} \lambda_n (1 + \lambda_n) J \frac{\partial P}{\partial \lambda_n},$$

$$J = \prod_{i=1}^{N} \prod_{j=i+1}^{N} |\lambda_j - \lambda_i|^3,$$

where $\lambda_n$ is related to $T_n$ by $\lambda_n = (1 - T_n)/T_n$, and $\beta$ is the symmetry index, $\beta = 1, 2$, or 4 for orthogonal, unitary, or symplectic class, respectively. For unitary class, which is the case we study here, the DMPK equation can be exactly solved [53]. The conductance distribution $P(\{\lambda_n\})$ can be further calculated from $P(\{T_n\})$, which was performed in Refs. [24,25]. Thus, the equivalence between the two models offers us great insights into the conductance properties of the chiral surface states in the quasi-1D regime.

Numerically, the conductance distributions of the chiral surface states have only been studied in Ref. [23] using the 2D directed network model. In the presence of strong surface disorder, the 2D directed network model is no longer valid [23]. It is an open question whether the conductance properties of the chiral surface states are still equivalent to that of the bulk-disordered quasi-1D wire in the quasi-1D regime. In the following, we investigate the effect of surface disorder on the conductance distributions of the surface states using the 3D tight-binding model under various disorder strengths.

We first present the results in the quasi-1D metal regime. Figure 5(a) shows the conductance distributions $P(\{\lambda_n\})$ in a quasi-1D system $30 \times 30 \times L_z$ at $E = -1.35$ with $\phi = \phi_0/3$, $t_z = 0.1$, and $W = 1$. We recall that the localization length of this system is $\xi = 65.3 \pm 2.1$, which has been calculated in Sec. III A. For $L_z = 6, 9, 14$, and $L_z \ll \xi$, the system is deeply in the metallic regime. As shown in the figure, $P(\{\lambda_n\})$ is well approximated by a Gaussian in this regime. We note that the widths of the distributions barely change with $L_z$ at small $L_z/\xi$. The variance of the conductance is 0.0637, 0.0692, and 0.0715 for $L_z = 6, 9$, and 14, respectively, which is close to the universal value 1/15 in the unitary class [53,57].

For the quasi-1D insulator regime, in Fig. 5(b), we plot the conductance distributions $P(\{\lambda_n\})$ in a quasi-1D system $21 \times 21 \times L_z$ at $E = -1.35$ with $\phi = \phi_0/3$, $t_z = 0.1$, and $W = 6$. The calculated localization length is $\xi = 2.66 \pm 0.02$ for this system. We choose $L_z = 25, 35$, and 45, which fulfills $L_z \gg \xi$, to plot the conductance distributions. As shown in the figure, $P(\{\lambda_n\})$ can be well fitted by log-normal distributions in this regime.

The conductance distribution is of particular interest in the crossover regime, where $\langle g \rangle \sim g^{1/2}$. Figure 6 represents the evolution of $P(\{\lambda_n\})$ in a quasi-1D system $L \times L \times L_z$ at $E = -1.35$ with $\phi = \phi_0/3$, $t_z = 0.1$ in the crossover regime. We choose two sets of parameters of transverse system sizes and disorder strengths. For all cases, the agreements between the two distributions are excellent. This validates the single-parameter scaling hypothesis in this surface-disordered system. The conductance distribution depends only on the average conductance, independent of details of the system. As the average conductance $\langle g \rangle$ decreases, $P(\{\lambda_n\})$ gradually deviates from the Gaussian distribution in the metallic regime. For $\langle g \rangle = 4/5$, only the $g > 1$ part can be approximated by the Gaussian function. At $\langle g \rangle = 1/2$, the distribution becomes highly asymmetric and there is a drastic change near $g = 1$. Finally, for $\langle g \rangle = 1/3$, the distribution develops a huge peak in the small $g$ region, driving the system towards the insulating regime. The peculiar forms of the conductance distributions in the crossover regime has also been observed in other systems [29,24,25,58] in the unitary class [59,60] which are indicated as continuous lines in Fig. 6. Therefore, our results suggest that the conductance properties of the chiral surface states are the same as that of a bulk-disordered quasi-1D wire in the quasi-1D regime, even in the presence of strong surface disorder.

Finally, it is worth noting that different from ordinary surface-disordered wire [61], the bulk of our system is insul-
IV. SUMMARY AND DISCUSSION

To summarize, we have investigated the effect of surface disorder on the chiral surface states of a 3D quantum Hall system. We find that in the weak disorder regime, the localization length in the $z$ direction decreases with the disorder strength as expected. However, after a critical disorder strength, which is of the order of the bandwidth, the localization length increases anomalously. As the disorder strength increases, the main weight of the surface state gradually moves from the outmost layer to the first inward layer. We explain the anomalous increase of the localization length by an effective model, which maps the strong disorder on the surface layer to the weak disorder on the first inward layer. Since surface disorder can be easily manipulated by adatom deposition, ion sputtering, and air exposure in experiments, it can be an effective way to control the behavior of the surface states in the $z$ direction.

We also investigate the effect of surface disorder on the conductance distributions $P(g)$ of the chiral surface states in the quasi-1D regime. We find that in the quasi-1D regime, the conductance distributions of the surface states are the same as that of a bulk-disordered quasi-1D wire in the unitary class. $P(g)$ is fully determined by the average conductance, independent of the surface disorder strength and the size of the system, in agreement with the single-parameter scaling hypothesis. Since the conductance can be directly measured in experiments, we expect our results can be verified by experiments in the future.

Throughout this work, the disorder is only added on the outmost sidewalls of the sample, the bulk is left clean. We have confirmed that the above conclusions still hold if we introduce weak disorder in the bulk, which is often the case in a realistic sample. The main effect of bulk disorder is to decrease the bulk band gap, hence increases the penetration depth of the surface states. It also decreases the localization length of the surface states in the $z$ direction. In the presence of bulk disorder, the conductance distribution $P(g)$ is still the only function of the average conductance and coincides with the DMPK results for a bulk-disordered quasi-1D wire in the unitary class.

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