Tunable Anderson Metal-insulator transition in quantum spin Hall insulators

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We study disorder effects in Bernevig-Hughes-Zhang (BHZ) model (unitary system), and find that Anderson transition of quantum spin Hall insulator (QSHI) is determined by model parameters. In contrast to the common belief that 2D unitary system scales to insulator except at certain critical points, we find, through calculations scaling properties of the localization length, level statistics, and participation ratio, that a possible exotic metallic phase emerges between QSHI and normal insulator phases in InAs/GaSb-type BHZ model. On the other hand, direct transition from QSHI to normal insulator is found in HgTe/CdTe-type BHZ model. Furthermore, we show that the metallic phase originates from the Berry phase and can survive both inside and outside the gap.

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I. INTRODUCTION

Topological insulators (TI) identified as a class of quantum state of matter have generated intensive interests recently. The two dimensional (2D) TI - quantum spin Hall insulator (QSHI), is characterized by odd pairs of counter propagate gapless edge states. The QSHI was firstly realized in HgTe/CdTe quantum well (QW) and subsequently in InAs/GaSb QW. These two experimentally realized QSHI systems can both be represented by the inverted bands Bernevig-Hughes-Zhang (BHZ) model but with different parameters. Specifically, the coupling strength between two inverted bands in InAs/GaSb QW is an order of magnitude smaller than that of HgTe/CdTe QW. Considering the remarkable parameter difference, one open question remains: whether this difference will have some physical consequences in these two QSHI systems.

The Anderson metal-insulator transition in 2D disorder system manifests as a lasting research interest in condensed matter physics. Generally, the disordered electron systems can be classified into three universality ensembles according to the random matrix theory. In the presence of time reversal symmetry (TRS), the system is classified as orthogonal ensemble if spin rotation symmetry is preserved; otherwise, it belongs to symplectic ensemble. In contrast, when the TRS is broken, the system turns into unitary ensemble. For TRS QSHI with Rashba spin orbital coupling (SOC), the system falls into the symplectic ensemble because spin rotation symmetry is broken. Oppositely, without Rashba SOC, QSHI is divided into two spin species of quantum anomalous Hall (QAH) systems, which belong to unitary ensemble. Previous studies on metal insulator transition in QSHI can be summarized into two paradigms: (i) for (symplectic) QSHI with Rashba SOC, it was found that TI and normal insulator (NI) phases are separated by a metallic phase (ii) for (unitary) QSHI without Rashba SOC, direct transition from TI to NI was discovered. Surprisingly, recently a crossover from weak localization to weak anti-localization (WAL) is suggested in BHZ model without Rashba SOC. Since WAL can add positive correction to β-function there is the possibility that a metallic phase might exist in the 2D unitary system (QSHI) with weak disorder, although that is against the traditional view.

In this paper, we study whether a metallic phase can exist between TI and NI phases in a unitary QSHI system. Starting from BHZ model Hamiltonian, we calculate localization length and two-terminal conductance numerically, and analyze the scaling behavior of the system. The main results are summarized in the phase diagrams in Fig. [1]. In all these phase diagrams, we find a metallic phase between TI and NI phases, in contrast to the common view of Anderson transition behavior in 2D unitary class. Furthermore, we find different parameters in BHZ model (unitary system) can lead to different Anderson transition behaviors. The transition from TI to metal is likely to exist in InAs/GaSb-type BHZ model but not in HgTe/CdTe-type BHZ model [see dash lines in Fig. [1(b)]. By employing the Berry phase, the parameter-dependent metallic phase can be well explained.

The rest of the paper is organized as follows. In Sec. II, we introduce the lattice model Hamiltonian and give the details of numerical simulations. In Sec. III, we show the main results by scaling of the localization length and scaling of the conductance. We discuss energy level statistics and participation ratios of eigenstates in In Sec. IV. In Sec. V, we discuss the phase diagram and interpret our numerical results by the Berry phase. In Sec.VI, a brief summary is presented.
\( L \) edge states. \( g \) is defined as \( 1/g = 1/g_L - 1/N \), with \( g_L \) the two-terminal conductance and \( N \) the number of propagating channels. The localization length \( \lambda_L \) of the sample is calculated by transfer matrix method with the sample’s length \( 10^6 \) to \( 10^7 \). The two-terminal conductance \( g_L \) at Fermi energy \( E_F \) is evaluated by Landauer-Büttiker formulation with considering a disordered middle region with size \( L \times L \) being coupling to two clean semi-infinite leads. In addition, we also investigate the energy level statistics as well as participation ratios. For simplicity, the parameters \( B = 1, C = 0, D = 0 \) and \( a = 1 \) are fixed in the rest of paper, where we have assumed the particle-hole symmetry \( (D = 0) \).

III. METAL INSULATOR TRANSITION

Firstly, we study \( \Lambda = \lambda_L/L \) versus disorder strength \( W \) by increasing mass from \( M = -0.1 \) to 0.5 at fixed Fermi energy \( E_F = 0 \), as shown in Fig. 2. These parameters resemble the InAs/GaSb QW \( k \cdot p \) parameters. Notably, we find TI-metal-NI transition in InAs/GaSb-type BHZ model (unitary system) by increasing mass \( M \). In NI phase with \( M < 0 \), \( \Lambda = \lambda_L/L \) monotonously decreases with increasing \( L \) in Fig. 2(a) which indicates all the states are localized. In contrast, when \( M = 0.05 \) in TI phase \( (M > 0) \), the system shows one critical (touching) point where \( \Lambda \) is independent of \( L \) [see Fig. 2(b)], which is consistent with the previous studies of 2D unitary system. Due to the inverted gap, TI is robust to weak disorder, and NI phase appears after a certain disorder strength \( W_c = 2.3 \pm 0.13 \). Therefore, this critical (touching) point indicates a direct transition from NI to TI. Surprisingly, in Fig. 2(c), when the mass \( M \) is increased to 0.38, the metallic phase (\( \Lambda \) increasing with \( L \)) appears between \( W_{c1} \approx 1.40 \) [see inset of Fig. 2(c)] and \( W_{c2} \approx 7.10 \). This metallic phase is contradict to the common behavior of 2D unitary class. The unitary system,
e.g. quantum Hall system, is scaled to localized states except at certain critical (touching) points. Moreover, upon further increasing \( M \), the metallic phase region becomes larger, i.e. for \( M = 0.5 \), the metallic phase remains in Fig. 2(d) between \( W_{c1} \approx 1.40 \) [see inset of Fig. 2(d)] and \( W_{c2} \approx 8.2 \). This peculiar metallic phase between TI and NI phases in InAs/GaSb-type BHZ model is the main finding of our paper.

Next, we analyze the one parameter scaling behavior of the renormalized localization length \( \Lambda = \lambda_L/L \) near the critical points of Fig. 2(c). According to finite size scaling law, all \( \Lambda \) are fitted to \( \Lambda(W,L) = \Lambda_c + \sum_{n=1}^{N} \alpha_n(W-W_c)^{\nu} + b_0 L^y \) near the critical point \( \nu = 28, 38 \) and \( b_0 \) are the fitting parameters. For convenience, we define \( \Lambda'(W,L) = \Lambda(W,L) - b_0 L^y \), with the same parameters as \( \Lambda \). The best fit is given by minimizing \( \chi^2 \) statistic \( \chi^2 = \sum_{n=1}^{N} (\Lambda_n - \Lambda(W_n,L_n))^2/\sigma_n^2 \), where \( N \) is the number of the data and \( \sigma_n \) is the error of the \( n \)th data. The finding of the metallic phase and the large critical exponent \( \nu \) (almost twice as large as that obtained previously) in Fig. 3(c) and (d) suggests the existence of a possible new universality class. We caution that the standard deviations (\( \chi^2/N \)) are 3.3 and 3.5 for Fig. 3(b) and (d), respectively, which are somewhat larger than the common value unity and even larger size computations are desirable to obtain a high precision critical exponent \( \nu \).

Up to now, we have found the metallic phase for small \( A = 0.28 \), which resemble the parameters of InAs/GaSb-type BHZ model. To compare with previous studies, it is necessary to investigate Anderson transition for large \( A \) cases, i.e. HgTe/CdTe-type BHZ model. In Fig. 4(a) and (b), where \( M = 0.38 \) and \( E_F = 0 \), \( A \) increases from 1 to 2.1, in the region of HgTe/CdTe-type model parameters. The other parameters are the same as those of Fig. 2(c). Compared with the case \( A = 0.28 \) [see Fig. 2(c)], the metallic phase disappears for \( A = 1 \) and \( A = 2.1 \) because \( \Lambda \) hardly changes with the size near the touching point [see Fig. 4(a) and (b)]. This direct transition from TI to NI (i.e. \( A = 1, 2.1 \)) is consistent with previous study in HgTe/CdTe-type BHZ model. Meanwhile, the localization length decreases rapidly with increasing \( A \) from 0.28 to 2.1. From the above results, it is natural to conclude that the existence of the metallic
phase is highly dependent on the magnitude of \( \Lambda \). To be specific, the transition TI-metal-NI in InAs/GaSb-type BHZ model is absent in HgTe/CdTe-type BHZ model.

Now we consider the influence of Fermi energy \( E_F \) on the metallic phase. In Fig. 4(c), when \( A = 0.28 \), \( M = 0.38 \), and \( E_F = 0.08 \) in the neighborhood of gap center, the transition TI-metal-NI remains almost the same as that of Fig. 2(c) with \( E_F = 0 \). When Fermi energy is moved outside the band gap \( E_g \approx 0.16 \), i.e. \( E_F = 0.17 \), the transition from metal to NI is still observed by scaling \( \Lambda \) and \( \langle g \rangle \) in Fig. 4(d). It is clear that \( \langle g \rangle \) and \( \Lambda \) increase with size of the system in metallic phase, decrease in insulator phase, and has a crossing point \( (W \approx 8) \) at the phase transition. To conclude, the localization length scaling and the conductance scaling suggest that the metallic phase could survive both inside and outside the band gap.

**IV. ENERGY LEVEL STATISTICS AND PARTICIPATION RATIO**

Furthermore, we have verified the existence of the metallic phase by studying the energy level statistics and evaluating the participation ratio of eigenstates. According to the random matrix theory, the delocalized and localized states can be characterized by the energy level statistics. In Fig. 4, the histograms of the level spacings are drawn at different energies \( E_F \). The sizes is \( 48 \times 48 \) with a periodical boundary condition on two directions, i.e., a torus geometry. In the energy region \( E_F = 0 \) to \( 0.2 \), the histograms [see Fig. 4(b)-(d)] and corresponding variances [see Fig. 5(a)] are very close to those of Wigner surmise of unitary ensemble \( p(s) = (32/\pi^2)s^2 \exp(-s^2) \). So, the level correlation is long ranged which indicates extend states may exist. However, near the top of the band \( (E = 8) \) [see Fig. 5(i)], the histogram is close to the Poisson distribution \( p(s) = \exp(-s) \), which implies that the states are uncorrelated and localized.

However, in the histograms of the level spacings, it is difficult to distinguish the critical point (or region) from the true metallic phase, because they are both close to Wigner surmise of the unitary class. In order to identify the true metallic phase, we test the larger sizes \( (L \times L = 128 \times 128) \) results at fixed energy \( E_F = 0 \) with different disorder strength \( W = 1 \) to 12. Then we fit the distributions to Wigner surmise \( p(s) = as^\alpha \exp(bs^3) \).
The model parameters are $A$ and $\beta$. The participation ratio characterized the spatial extension of the eigenstates. Next, let’s come to investigate the participation ratio under different disorder strength. The participation ratio is defined as $R = \sum_{\lambda} \langle \chi_{\lambda} | \chi_{\lambda} \rangle$. In this case, the level correlation is finite ranged, which manifests as a crossing over from (long ranged correlated) Poisson statistics to (uncorrelated) Poisson statistics. For $W = 1$ and $W = 12$ [see Fig. 6(a) and (f)], the level spacings clearly deviated from the Wigner surmise of the unitary ensemble for whole $s$ region and the energy levels will become totally uncorrelated in thermodynamic limit, identifying an insulating phase. In conclusion, the level statistics results strongly support the existence of a metallic phase between $W = 4$ and $W = 6$ at $E_F = 0$. This is coincident with the region indicated by finite size scaling results of localization length (see Fig. 1).

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\[ \sum_{i=1}^{N} |a_i|^4/(N \sum_{i=1}^{N} |a_i|^2) \] where \( a_i \) is the wave function at lattices \( i \) and \( N \) is the number of the lattice. \( R \) has its maximum 1 for same Bloch wave, reaches a finite value typical around 1/3 for an disordered extended state, and approaches \( \sim 1/N \) for a localized state. In Fig. 7(b) and (c), the (highly possible) extended states characterized by the peaks \( R \approx 0.6 \) are found near the bulk gap at \( W = 1 \), and then come into the bulk gap with increasing the disorder strength \( W = 3 \). As a result, the metallic phase in the gap indeed comes from the extended states near the gap, which originates from the nearly \( \pi \) Berry phase. At last, the peak of \( R \) diminishes with increasing the disorder strength, see Fig. 7(d)-(f) which indicates that the states are localized at \( W = 14 \) (\( R < 1/3 \)).

V. PHASE DIAGRAM AND DISCUSSION

We summarize our results into three phase diagrams: \( W-M, W-A, \) and \( W-E_F \), as shown in Fig. 1. In Fig. 1(a), the metallic phase emerges from TI phase at \( M \simeq 0.1 \) and expands with increasing \( M \) from 0.1 to 1. On the other hand, in Fig. 1(b), the metallic phase exists for small \( A \) cases and disappears for \( A > 0.56 \). In other word, the transition TI-metal-NI can exist in InAs/GaSb-type BHZ model but not in HgTe/CdTe-type BHZ model. In the present case, the detailed analysis of symmetry classes and Berry phases can help us to understand the peculiar metallic phase in inverted band BHZ model. We first analyze the symmetry classes of the BHZ model. The spin-\( \uparrow \) part of BHZ Hamiltonian in momentum space is \( H_0(k) = A(k_x \tau_x + k_y \tau_y) + (M - Bk^2)\tau_z \), where \( A, B, M \) and \( \tau \) have the same meaning as in Eq. 2. When the mass term \( M - Bk^2 \) = 0, the system satisfies pseudo-time reversal symmetry, i.e. \( H_0(k_F) = \tau_y H_0^*(-k_F) \tau_y \), which is similar to the massless Dirac particles in graphene. Therefore, the system is approximate symmetrical and shows WAL in the region near \( M - Bk^2_F = 0.0 \). On the contrary, when \( |M - Bk^2_F| >> \sqrt{A |k_x + ik_y|} \), the two orbital bands are nearly decoupled, thus the system belongs to orthogonal ensemble approximately and shows weak localization. So the existence of the metallic phase is dependent on the system parameters. Moreover, the Berry phase of the BHZ model at Fermi energy \( E_F \) reads:

\[ \gamma(E_F) = (1 - \frac{(M - Bk^2_F)}{\sqrt{A^2 + (M - Bk^2_F)^2}})\pi, \]

where \( k_F \) is the momentum at \( E_F \). The Berry phase \( \gamma \) monotonously increases with \( k_F \), rising from zero. \( \gamma = 0 \) at \( k_F = 0 \), \( \gamma = \pi \) at \( k_F = \sqrt{M/B} \), and \( \gamma \to 2\pi \) while \( k_F \) tends to \( \infty \). Since \( \gamma \) can vary from 0 to \( 2\pi \), the system can show both WAL and weak localization which depends on the parameters. While \( M/B >> A^2/B^2 \), \( k_g = \sqrt{\frac{M}{B} - \frac{A^2}{2B^2}} \sim \sqrt{M/B} \) where \( k_g \) is the momentum at the conduction band bottom and the valence band top, and then the Berry phase \( \gamma \approx \pi \). In this case, the system shows WAL and the metallic phase exists between TI and NI phases (see Fig. 1). For the case of InAs/GaSb-type BHZ model, i.e. \( A = 0.28, B = 1 \), and \( M = 0.38 \), \( M/B >> A^2/B^2 \) is well satisfied, the metallic phase appears consequently. Oppositely, for HgTe/CdTe type model, i.e. \( A = 1, B = 1 \), and \( M = 0.38 \) with \( M/B < A^2/B^2 \), \( k_g = 0 \) which is far away from \( \sqrt{M/B} \). At \( k_g = 0 \), the Berry phase \( \gamma = 0 \), which leads the weak localization behavior and the disappearance of the metallic phase.

VI. SUMMARY

We investigate Anderson metal-insulator transition in QSHI and find different localization behaviors depending on model parameters. Notably, the transition TI-metal-NI likely exists in InAs/GaSb-type systems but not in HgTe/CdTe-type systems. The peculiar metallic phase, which originates from the Berry phase \( \pi \) near the band gap, contradicts to the common view of Anderson transition behavior of 2D unitary class.

VII. ACKNOWLEDGEMENTS

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The dimensionless parameters $A = 0.28$, $B = 1$, $C = 0$, $D = 0$, $M = -0.1$ to 0.5 correspond to $A = 37\text{meV}\cdot\text{nm}$, $B = -660.8\text{meV}\cdot\text{nm}$, $C = 0$, $D = 0$ and $M = 2.6\text{meV}$ to $-13.2\text{meV}$, with the lattice constant $a = 5\text{nm}$. They are InAs/GaSb-type $k \cdot p$ parameters because $A$ is about an order of magnitude smaller than that of HgTe/CdTe-type.

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