Paradoxical extension of the edge states across the topological phase transition due to emergent approximate chiral symmetry in a quantum anomalous Hall system

Denis R. Cândido*, Maxim Kharitonov*, J. Carlos Egues†, Ewelina M. Hankiewicz‡

*These authors contributed equally
†Instituto de Física de São Carlos, Universidade de São Paulo, 13560-970, São Carlos, São Paulo, Brazil
‡Institute for Theoretical Physics and Astrophysics, University of Würzburg, 97074 Würzburg, Germany

We present a paradoxical finding that, in the vicinity of a topological phase transition in a quantum anomalous Hall system (Chern insulator), topology nearly always (except when the system obeys charge-conjugation symmetry) results in a significant extension of the edge-state structure beyond the minimal one required to satisfy the Chern numbers. The effect arises from the universal gapless linear-in-momentum Hamiltonian of the nodal semimetal describing the system right at the phase transition, whose form is enforced by the change of the Chern number. Its emergent approximate chiral symmetry results in an edge-state band in the vicinity of the node, in the region of momenta where such form is dominant. Upon opening the gap, this edge-state band is modified in the gap region, becoming “protected” (connected to the valence bulk band with one end and conduction band with the other) in the topologically nontrivial phase and “nonprotected” (connected to either the valence or conduction band with both ends) in the trivial phase. The edge-state band persists in the latter as long as the gap is small enough.

Introduction and main result. In quantum anomalous Hall (QAH) systems (also known as Chern insulators)1–4, the topological Chern number C of an insulating phase defines, via bulk-boundary correspondence2,4, the number of the edge-state bands that connect the valence and conduction bulk bands. This is the only characteristic of the edge states required by quantum Hall (QH) topology. Such states are topologically protected in the sense that they cannot disappear under continuous deformations of the Hamiltonian without closing the gap in the bulk spectrum.

One could define minimal edge-state structures that are sufficient to satisfy a given Chern number. In particular, in the topologically nontrivial (TnT) phase with C = 1, one topologically protected edge-state band, having minimal extent in momentum space just enough to connect the valence and conduction bands (for more common band structures, this is typically the region of momenta dominated by the bulk gap), is sufficient. In the topologically trivial (TT) phase with C = 0, no edge states at all are required. No edge states are also required at the topological phase transition (TPT) between the TT and TnT phases, when the gap closes and the system is a semimetal, since C is not even well-defined there.

In principle, topologically nonprotected edge-state bands that are connected to either the valence or conduction band with both ends could additionally exist. Also, topologically protected edge-state bands could extend beyond the gap region. Such additional edge-state structures are not required by QH topology, but neither are they prohibited.

In this work, we present a paradoxical finding that, in the vicinity of a TPT in QAH system, QH topology nearly always results in a significant extension of the edge-state structure beyond the minimal one required to satisfy the Chern numbers, described above. This generic behavior is illustrated in Fig. 1 with the quadratic model, to be presented below, which describes one block of the Bernevig-Hughes-Zhang (BHZ) model5 of a quantum spin Hall (QSH) system6–7. This behavior has previously been noticed8 in the BHZ model, but remained unexplained.

Applying the ideas recently formulated in Ref. 9, we show that this extension of the edge-state structure originates from the emergent approximate chiral symmetry of the universal gapless linear-in-momentum low-energy Hamiltonian of the nodal semimetal describing the system right at the TPT, which in its simplest form reads

$$\hat{H}_0(p) = v(\tau_x p_x + \tau_y p_y),$$

(1)

where \(\tau_{x,y}\) are Pauli matrices in the space defined below and \(v\) is the velocity of its linear spectrum \(\pm v|p|\), \(p = (p_x, p_y)\). This results in an edge-state band that exists [Fig. 1(b)] at the TPT on one side of the node (at least) in the region \(|p_x| \lesssim p^*\) of momenta \(p_x\) along the \(y = 0\) edge, where such asymptotic form of the Hamiltonian is dominant; \(p^*\) is the scale, where higher-order-in-momentum terms in the asymptotic expansion of the full Hamiltonian become comparable to the linear ones. Upon opening a small gap \(\Delta\), such that \(p_\Delta = |\Delta|/v \ll p^*\), the edge-state band is modified only in the smaller region \(|p_x| \lesssim p_\Delta\) dominated by the gap, in accord with QH topology. In the TT phase \([C = 0, \text{Fig. 1(a)}]\), the edge-state band exists in the region \(p_\Delta \lesssim |p_x| \lesssim p^*\) and remains topologically nonprotected, connected to the valence (in the case of quadratic model presented in Fig. 1) band with both ends without crossing the gap. In the TnT phase \([C = 1, \text{Fig. 1(c)}]\), the edge-state band becomes topologically protected, connected to the valence band with one end and conduction band with the other.
FIG. 1: Edge states (blue) of a quadratic model (6) and (7) of a QAH system in the vicinity (\(p_\Delta \ll p^* \sim \kappa = v/\sqrt{\beta_a \beta_b}\)) of the TPT. At smaller momenta, the edge-state structure agrees with that (dashed red) of the low-energy linear model [Eqs. (2), (3), and (8), Fig. 2]. Grey-shaded regions denote the continua of bulk states. (a),(b),(c) Due to the approximate chiral symmetry of the linear model, in the general case \(\beta_a \neq \beta_b\) of unequal curvatures \(\beta_a, b\) of the conductance and valence bands, the edge-state structure is extended beyond the minimal one required to satisfy the Chern numbers. (d),(e),(f) Only in the exceptional case \(\beta_a = \beta_b\), when the system obeys charge-conjugation symmetry, the minimal edge-state structure is realized. Graphs (a),(b),(c) are plotted for \(\beta_a/\beta_b = 10\). Graphs (a),(c),(d),(f) are plotted for \(\kappa/\kappa_\Delta = 3\sqrt{10}\).

crossing the gap in the region \(|p_x| \lesssim p_\Delta\), but also extending well beyond it to the region \(p_\Delta \lesssim |p_x| \lesssim p^*\).

Even though this extension of the edge-state structure is not topologically protected, it is nearly always present, i.e., for all forms of the low-energy model, except when it obeys charge-conjugation symmetry [Fig. 1(d),(e),(f)], which is an exceptional case that can likely be achieved only by accident or fine-tuning. Only in this case, the edge-state structure is minimal in the sense described above.

Our finding is quite paradoxical because the form (1) of the nodal semimetal Hamiltonian at the TPT is ultimately enforced by QH topology, to ensure the change of the Chern number across the TPT. This form, due to its approximate chiral symmetry, generates the extension of the edge-state structure, which is, however, not required to satisfy the Chern numbers in either the TT (\(C = 0\)) or TuT (\(C = 1\)) phase.

Low-energy Hamiltonian in the vicinity of a topological phase transition. We consider a QAH system, i.e., a 2D band insulator with broken time reversal symmetry, but no orbital effect of the magnetic field. Such system belongs to class A of the general classification scheme of topological systems and is characterized by an integer \(\mathbb{Z}\) bulk topological invariant well known as the Chern number.

We consider the vicinity of a TPT in a QAH system. At the phase transition, two electron states, to be denoted \(a\) and \(b\), become degenerate at some point in the Brillouin zone, making the system gapless. The low-energy linear-in-momentum Hamiltonian for the wave function \(\psi = (\psi_a, \psi_b)^T\) in the subspace of these two states can be written in its simplest form as

\[
\hat{H}(p) = v (\tau_x p_x + \tau_y p_y) + \Delta \tau_z,
\]

where \(\tau_x, \tau_y, \tau_z\) are the Pauli matrices and \(p = (p_x, p_y)\) is the momentum deviation from the degeneracy point. In general, several additional terms could be present. In Supplemental Material (SM)\(^{10}\), we demonstrate that our findings for the simplest Hamiltonian \(\hat{H}(p)\) presented below also hold for the most general form of the linear Hamiltonian.

The two insulating QAH phases correspond to two signs of the gap \(\Delta > 0\) and \(\Delta < 0\) and have a difference \(C_{\Delta < 0} - C_{\Delta > 0} = 1\) of the Chern numbers \(C_{\Delta > 0}; \Delta = 0\) is the TPT point, where the system is gapless nodal semimetal, described by the Hamiltonian \(\hat{H}_0(p) = \hat{H}(p)|_{\Delta = 0}\) [Eq. (1)]. We assume that one of the phases is TT with a zero Chern number, i.e., that possible full Chern numbers are \((C_{\Delta < 0}, C_{\Delta > 0}) = (1, 0)\) or \((0, -1)\).

The Hamiltonian (2) is valid at momenta \(p = |p| \lesssim p^*\) not exceeding the scale \(p^*\) defined above. Accordingly, the gap must also be small enough, so that \(p_\Delta \lesssim p^*\).

General boundary condition. Next, we supplement the low-energy Hamiltonian \(\hat{H}(p)\) [Eq. (2)] with the boundary condition (BC) of the most general form, describing termination of the sample, without any assumptions about the microscopic structure of the boundary. Such form is constrained by the only fundamental requirement that the probability current perpendicular to the boundary must vanish. Such BC has recently been derived\(^{11}\) in Ref. 9 for the gapless Hamiltonian \(\hat{H}_0(p)\) [Eq. (1)]. Since the current operator \(\hat{j} = \partial_\tau \hat{H}(p) = v (\tau_x, \tau_y)\) does not depend on \(\Delta\) at all, the BC remains exactly the same for finite \(\Delta\). Throughout the paper, we consider the sample occupying the half-plane \(y > 0\). The BC for the \(y = 0\) edge\(^{12}\) reads

\[
\psi_a(x, y = 0) = \sin \frac{\theta}{2} \psi_b(x, y = 0) \cos \frac{\theta}{2} = 0.
\]

All unique forms of the BC are parameterized by the angle \(\theta\) covering the full circle, shown in Fig. 2(d).

Generic edge-state structure. The edge states for the Hamiltonian (2) and BC (3) can be calculated analytically and are shown in Fig. 2. All possible forms are parameterized by the angle \(\theta\) and represent the generic edge-state structure in the vicinity of a TPT of QAH system, see also SM\(^{10}\). For every value of \(\theta\) except \(\pm \frac{\pi}{2}\) (to be discussed separately below), there exists one edge-state band

\[
\mathcal{E}(p_x) = v p_x \sin \theta + \Delta \cos \theta
\]

for any value of the gap \(\Delta\), at \(p_x > p^m_\Delta(\theta)\) for \(\theta \in \Theta_\Delta = (-\frac{\pi}{2}, \frac{\pi}{2})\) and at \(p_x < p^m_\Delta(\theta)\) for \(\theta \in \Theta_\Delta = (\frac{\pi}{2}, \frac{3\pi}{2})\).

\((v p^m_x(\theta), e^m(\theta)) = \Delta (\tan \theta, 1/\cos \theta)\) is the merging point
of the edge-state dispersion relation (4) with the boundaries ±√((vp₂)² + Δ₂²) of the continua of the bulk states.

Therefore, as the key property, the edge-state structure in the vicinity of the TPT in a QAH system is nearly always (i.e., for all θ ≠ ±π/2) extended beyond the minimal one required to satisfy the Chern numbers. For the model (1) and (3) with Δ = 0 [Fig. 2(b)], these edge states have recently been found and studied in Ref. 9. Applying the ideas expressed therein, below we demonstrate that this extension of the edge states can be explained in terms of chiral symmetry.

Edge states at the topological phase transition due to chiral symmetry. Chiral symmetry is one of the three main symmetries (along with time-reversal and charge-conjugation) that give rise to topological behavior. A bulk Hamiltonian $\mathcal{H}(p)$ satisfies chiral symmetry, if there exists a unitary operator $\hat{S}$ under which it changes its sign, $\hat{S}\mathcal{H}(p)\hat{S}^\dagger = -\mathcal{H}(p)$.

In 2D, chiral symmetry allows for the existence of gapless topological semimetals with flat edge-state bands at zero energy $\epsilon = 0$. We notice that the gapless bulk Hamiltonian $\mathcal{H}_0(p)$ [Eq. (1)] at the TPT obeys chiral symmetry with $\hat{S} = \tau_z$. An important requirement for the topologically protected $\epsilon = 0$ edge states to exist is that the system with an edge must respect chiral symmetry. For a low-energy model, this means that not only the bulk Hamiltonian but also the BC must respect chiral symmetry. For the general BC (3), there are only two discrete cases

$$\psi_b(x, y = 0) = 0 \text{ or } \psi_a(x, y = 0) = 0 \quad (5)$$

with $\theta = 0$ or $\theta = \pi$, respectively, that obey chiral symmetry.

The model with the bulk Hamiltonian (1) and one of the BCs (5) represents a chiral-symmetric 2D topological semimetal. For each of the chiral-symmetric BCs (5), there is a flat edge-state band at $\epsilon = 0$ on one side of the node, for $p_x > 0$ and $p_x < 0$, respectively [Fig. 2(b)], ensured by the well-defined topological invariant of the node, the winding number 1.

The low-energy model of a QAH system in the vicinity of a TPT with the Hamiltonian (2) and BC (3) does not generally have exact chiral symmetry: in $\hat{H}(p)$, the gap term $\Delta\tau_z$ breaks chiral symmetry $\hat{S} = \tau_z$ and the BC generally differs from one of the chiral-symmetric forms (5). However, as demonstrated in Ref. 9, exact chiral symmetry is not required for the edge states induced by it to persist due to their stability property. Upon breaking chiral symmetry, the edge-state bands depart from $\epsilon = 0$, but continue to persist as long as chiral-symmetric parts of the Hamiltonian and BCs are dominant. Accordingly, the concept of a stability region was introduced therein, as the region in the parameter space of chiral-asymmetric terms where the edge states persist.

At the TPT $\Delta = 0$ [Fig. 2(b)], the edge-state dispersion relation (4) reads $\mathcal{E}(p_x)|_{\Delta = 0} = vp_x \sin \theta$. The circle of $\theta$ consists of two stability regions $\Theta_{a,b} = (-\pi, \pi)\setminus(\pi, \frac{3\pi}{2})$ and $\Theta_{a,b} = (\pi, \frac{3\pi}{2})\setminus(\frac{\pi}{2}, \frac{3\pi}{2})$, for which the edge-state band is located at $p_x \gg 0$, respectively. The regions $\Theta_{a,b}$ contain the chiral-symmetric points $\theta = 0$ and $\theta = \pi$, respectively, corresponding to the BCs (5). As $\theta$ deviates from one of these points, the edge-state band deviates from $\epsilon = 0$ acquiring a finite slope. The edge-state band disappears by merging with the bulk bands only upon reaching $\theta = \pm\pi/2$ points. The stability regions $\Theta_{a,b}$ are thus separated only by two points $\theta = \pm\pi/2$ and the edge states persist even for significant deviations from chiral symmetry.

To summarize this part, right at the TPT of a QAH system, when the system is a nodal semimetal, an edge-state band [Fig. 2(b)] nearly always (i.e., for all values of the parameter $\theta$ in the BC (3), except $\pm\pi/2$) exists (at least) in the region $|p_x| \lesssim p^*$, where the linear terms of $\mathcal{H}_0(p)$ are dominant in the full Hamiltonian. This band can be attributed to the approximate chiral symmetry of the model (1) and (3). This band in not required by QH topology and is therefore an extension of the minimal edge-state structure.

![FIG. 2: Generic edge-state structure [Eq. (4)] in the vicinity of a TPT in a QAH system, calculated for the simplest form (2) of the low-energy linear-in-momentum Hamiltonian with the most general BC (3); see SM 10 for the most general form of the Hamiltonian. Due to the approximate chiral symmetry of the model, for every value of the parameter $\theta$ of the BC (3) except $\pm\pi/2$, when the system satisfies charge-conjugation symmetry, the edge-state structure is extended at the TPT $\Delta = 0$, (a) and in both TT and TnT phases $\Delta \geq 0$, (a),(c)](image-url)
Modification of the edge-state band by the gap. Introducing a small gap $\Delta$, such that $p_\Delta \ll p^*$, modifies this edge-state band only in the smaller region $|p_x| \lesssim p_\Delta$ dominated by the gap, in accord with QH topology. Indeed, as Figs. 2(a) and (c) show, in this region, the edge-state behavior is crucially sensitive to the sign of the gap, i.e., to which QAH phase the system is in. The numbers of the edge-state bands crossing the gap\(^4\) with the sign of their velocities $E_{p_x}(p_\pm) \sim v \sin \theta$ are: 0 and $+1$ for $\Delta \gtrsim 0$, respectively, if $\theta \in (0, \pi)$, and $-1$ and 0 for $\Delta \lesssim 0$, respectively, if $\theta \in (\pi, 2\pi)$. The difference of these numbers for $\Delta \gtrsim 0$ at each value of $\theta$ is in full accord with the difference $C_{\Delta<0} - C_{\Delta>0} = 1$ of the Chern numbers, manifesting the bulk-boundary correspondence of a QAH system.

However, also for a finite gap, in the region $p_\Delta \lesssim |p_x| \lesssim p^*$, the edge states are still determined by the linear chiral-symmetric part $H_0(p)$ [Eq. (1)] of the Hamiltonian $H(p)$ [Eq. (2)], which is dominant there. As seen from Figs. 2(a),(b),(c), the edge-state structure in the region $p_\Delta \lesssim |p_x| \lesssim p^*$ is the same regardless of the presence of the gap and its sign and represents the extension beyond the minimal structure required to satisfy the Chern numbers.

The cases $\theta = \pm \frac{\pi}{2}$ of charge-conjugation symmetry. For $\theta = \pm \frac{\pi}{2}$, there is an edge-state band (4) only in one of the insulating phases $\Delta \lesssim 0$, respectively, while there are no edge states at the TPT $\Delta = 0$ and in the other insulating phase $\Delta \gtrsim 0$. Only in these cases of $\theta$ the minimal edge-state structure is realized. In SM\(^{10}\), we demonstrate that the bulk Hamiltonian $\hat{H}(p)$ [Eq. (2)] with the gap and the BC (3) at $\theta = \pm \frac{\pi}{2}$ satisfy charge-conjugation symmetry. Therefore, for $\theta = \pm \frac{\pi}{2}$, the system with an edge obeys charge-conjugation symmetry. Thus, interestingly, the only cases of the general BC (3), in which the edge states at the TPT $\Delta = 0$ [Fig. 2(b)] induced by chiral symmetry are absent, are the ones that have charge-conjugation symmetry. This can be understood as follows. For charge-conjugation symmetry, the edge-state spectrum has to satisfy $E(p_x) = -E(-p_x)$, which is incompatible with the property that chiral symmetry induces only one edge-state band on either side ($p_x > 0$ or $p_x < 0$) of a linear node.

Edge states of the quadratic model. Above, we have established the generic behavior of the edge states (Fig. 2) of a QAH system in the vicinity of a TPT using the universal low-energy model with the linear-in-momentum Hamiltonian, given by Eqs. (2) and (3) in its simplest form and in SM\(^{10}\) in its most general form. Any “full” model of a QAH system with an explicitly defined behavior at all momenta and properties of the boundary will asymptotically be described by this low-energy model in the vicinity of the TPT. The information about both the band structure of the bulk Hamiltonian away from the node and properties of the boundary will be fully contained in the BC of the low-energy model.

We demonstrate this point explicitly by considering the following QAH Hamiltonian

$$\hat{H}_2(p) = \begin{pmatrix} \Delta + \beta_\alpha p^2 & vp_- \\ vp_+ & -\Delta - \beta_\beta p^2 \end{pmatrix}, \quad p_{\pm} = p_x \pm ip_y, \quad (6)$$

with momenta taking all values up to infinity. One can recognize this model as one block of the BHZ model\(^5\). In addition to $\hat{H}(p)$ [Eq. (2)], this Hamiltonian contains diagonal quadratic terms $\beta_{\alpha,\beta} p^2$ with the curvatures $\beta_{\alpha,\beta} > 0$. These terms fully specify the topology, making the Chern number $C$ well defined. The phases $\Delta \gtrsim 0$ are TT and TnT with $C = 0, 1$, respectively. We consider “hard-wall” BCs\(^{15}\)

$$\psi_a(x, y = 0) = 0, \quad \psi_b(x, y = 0) = 0 \quad (7)$$

for the Hamiltonian (6).

The linearized Hamiltonian $\hat{H}(p)$ is obtained from $\hat{H}_2(p)$ just by neglecting the quadratic terms. The BC of the form (3) for the linearized Hamiltonian is derived in SM\(^{10}\). As a result, the quadratic model of Eqs. (6) and (7) is described asymptotically in the vicinity of the TPT by the linear model of Eqs. (2) and (3), with the angle $\theta$ of the BC determined by the ratio of the curvatures as

$$\tan^2 \frac{\theta}{2} = \sqrt{\beta_a/\beta_b}. \quad (8)$$

As $\beta_a/\beta_b$ spans $(0, +\infty)$, the angle $\theta$ spans the half-circle $(0, \pi)$; i.e., in this particular model, only half of the possible forms of the general BC (3) can be realized. The BC (3) becomes chiral-symmetric [Eq. (5)] only asymptotically in the limits $\beta_a/\beta_b \rightarrow 0, +\infty$, i.e., for strong particle-hole asymmetry.

The edge states for the quadratic model of Eqs. (6) and (7) can actually be found analytically. It turns out that its exact edge-state spectrum is given\(^{16}\) by that of the linear model with $\theta$ given by Eq. (8). For $\beta_a > \beta_b$, the exact edge-state band, shown in Fig. 1, exists in the interval $p_x^{m-} < p_x < p_x^{m+}$, where

$$p_x^{m \pm} = \frac{x \beta_a - \beta_b}{2 \beta_a + \beta_b} \left(-1 \pm \sqrt{1 - \frac{8 \Delta}{v^2} \frac{\beta_a \beta_b (\beta_a + \beta_b)}{(\beta_a - \beta_b)^2}}\right) \quad (9)$$

with $x = v/\sqrt{\beta_a/\beta_b}$ are the merging points with the bulk spectrum of Eq. (6). The merging points $p_x^{m-}$ at larger momenta can be used to define the scale $p^* \equiv |p_x^{m-}|$ of validity of the linear model. For $p_\Delta \ll x$ and not too small $\beta_a - \beta_b$, $p_x^{m-} \approx -x \frac{\Delta}{\beta_a + \beta_b} \sim x$.

We see that, indeed, for a small gap ($p_\Delta \ll p^*$), the exact edge-state behavior of the quadratic model at smaller momenta $|p_x| \ll p^*$ is in full accord with that of the linear model. For any value $\beta_a/\beta_b \neq 1$, the edge-state structure of the quadratic model in the vicinity of the TPT is extended beyond the minimal one, Figs. 1(a),(b),(c). Additionally, the well-defined merging point $p_x^{m-}$ at larger momenta explicitly shows that the edge-state behavior is in agreement with QH topology. In the TnT [Fig. 1(c)] and TT [Fig. 1(a)] phase, the edge-state band is topologically protected and nonprotected,
respectively. Upon increasing the gap in the TT phase, the merging points \( p_{\pm}^m \) come closer to each other and the edge-state band eventually disappears at \( p_\Delta \sim \kappa \).

For \( \beta_a = \beta_b \), Figs. 1(d),(e),(f), the quadratic model obeys charge-conjugation symmetry \(^{10}\) and the edge states exist only in the TnT phase in the gap region, realizing the minimal edge-state structure.

**Relation to real systems.** Having demonstrated in SM the extension effect of the edge-state structure for the most general low-energy model, we expect it to be widespread in real QAH systems, and also in QSH systems, at least when coupling between the Kramers blocks is weak\(^{17}\). In SM, we demonstrate that the effect is quite pronounced for the parameters of the BHZ model describing HgTe quantum wells.

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10. See Supplemental Material at [URL], which includes Refs. 2,4, for the most general form of the low-energy linear-in-momentum model of the topological phase transition of a quantum anomalous Hall system and its analysis in terms of chiral and charge-conjugation symmetries and for the derivation of the low-energy boundary condition (9) from the quadratic model [Eqs. (6) and (7)].
11. A mathematically equivalent result for a 1D gapped system was obtained earlier in M. T. Ahari, G. Ortiz, and B. Seradjeh, Am. J. Phys. 84, 858 (2016).
12. Due to axial rotation symmetry of the Hamiltonian \( \hat{H}(p) \) [Eq. (2)], the edge-state spectrum will be the same for any orientation of the edge.
13. The regions \( \Theta_{a,b} \) are labelled according to the dominant character of the wave function, \(|\psi_a| \gtrsim |\psi_b|\), respectively.
14. We assume that the edge states eventually merge outside of the region \(|p_x| \lesssim p^*\) of validity of the linear model with those bulk bands to which they are closest, as is the case, e.g., for the quadratic model (6) in Fig. 1.
15. Such BCs describe, for example, an interface with the TT phase of the model (6) with an infinite gap \( \Delta \rightarrow +\infty \).
16. We believe this is an accidental property of this model, since, in general, agreement can be expected only asymptotically.
17. If a QSH system possesses additional reflection symmetry along the direction perpendicular to the quasi-2D sample, such as the original BHZ model\(^{5}\), then it decouples into two QAH systems and our results apply directly. If there is no exact reflection symmetry, our results should still apply at least when the effect of reflection-symmetry breaking is weak. Generalization of our approach to stronger coupling should be possible.
Supplemental Material: Paradoxical extension of the edge states across the topological phase transition due to emergent approximate chiral symmetry in a quantum anomalous Hall system

Maxim Kharitonov\textsuperscript{1}, Denis R. Cândido\textsuperscript{2}, J. Carlos Egues\textsuperscript{2}, Ewelina M. Hankiewicz\textsuperscript{1}
\textsuperscript{1}Institute for Theoretical Physics and Astrophysics, University of Würzburg, 97074 Würzburg, Germany
\textsuperscript{2}Instituto de Física de São Carlos, Universidade de São Paulo, 13560-970, São Carlos, São Paulo, Brazil

I. MOST GENERAL LINEAR MODEL

Here, we demonstrate that the main claim of the paper, that the edge-state structure in the vicinity of the TPT in a QAH system is nearly always significantly extended beyond the minimal one required to satisfy the Chern numbers, is valid not only for the simplest form (2) of the linear Hamiltonian, but also for its most general form.

A. General bulk Hamiltonian, convenient basis

The most general 2D Hamiltonian up to the linear order in momentum for a two-component wave function, describing the vicinity of a TPT of a QAH system with no assumed symmetries, has the form

\[ \hat{H}(\mathbf{p}) = \sum_{\alpha=0,x,y,z} \tau_\alpha (\varepsilon_\alpha + v_{\alpha x} p_x + v_{\alpha y} p_y), \]  

(S1)

with 4 real energy parameters \( \varepsilon_\alpha \) and 8 real velocity parameters \( v_{\alpha x} \) and \( v_{\alpha y} \), i.e., with 12 real parameters, out of which \( \varepsilon_0 \) at \( \tau_0 \) is an inconsequential overall energy. Here, \( \tau_\alpha \) are the unity and Pauli matrices in the arbitrary initial basis of the two electron states and \( p_{x,y} \) are the cartesian momentum components in the arbitrary initial coordinate basis\textsuperscript{1}. Additionally, the orientation of the edge relative to the initial coordinate axes is described by one angle. And so, the edge-state problem is described by 12 real parameters: 11 relevant parameters of the bulk Hamiltonian and the angle specifying the orientation of the edge.

There is freedom in the independent choice of the wave-function \( \hat{\psi} = (\psi_a, \psi_b)^T \) and momentum \( \mathbf{p} = (p_x, p_y) \) bases. The wave-function basis has 3 real parameters of the SU(2) transformation matrix \( \hat{U} \),

\[ \hat{\psi} \rightarrow \hat{U} \hat{\psi}. \]

The momentum basis has one angle parameterizing the rotation matrix \( \hat{R} \) and 2 parameters \( \mathbf{p}_0 = (p_{x0}, p_{y0}) \) describing the choice of the origin,

\[ \mathbf{p} \rightarrow \hat{R} \mathbf{p} + \mathbf{p}_0. \]

We exploit these 6 free real parameters to bring the most general Hamiltonian (S1) to the most convenient form for the analysis of the BC and edge-state problem.

First, we use the angle of the rotation matrix \( \hat{R} \) to orient the edge as \( y = 0 \). Next, we use 2 of the 3 parameters of the SU(2) matrix \( \hat{U} \) to bring the matrix at \( p_y \) momentum perpendicular to the edge \( y = 0 \) to the diagonal form (containing only \( \tau_{0,z} \) and no \( \tau_{x,y} \)). After this, the Hamiltonian in this new basis takes the form

\[ \hat{H}(\mathbf{p}) = \tau_0 (v_{0x} p_x + v_{0y} p_y + \varepsilon_0) + \tau_z (v_{zx} p_x + v_{zy} p_y + \varepsilon_z) + \tau_y (v_{yx} p_x + \varepsilon_y) + \tau_y (v_{yx} p_x + \varepsilon_y). \]

(In order not to overcomplicate the notation and since we are interested only in the final convenient form of the Hamiltonian, we will preserve the same notation in all bases; this should not lead to confusion.) Next we use the remaining 3rd parameter of \( \hat{U} \) to eliminate the velocity \( v_{xx} \), which brings the Hamiltonian to the form

\[ \hat{H}(\mathbf{p}) = \tau_0 (v_{0x} p_x + v_{0y} p_y + \varepsilon_0) + \tau_y (v_{yx} p_x + \varepsilon_y) + \tau_z (v_{zx} p_x + v_{zy} p_y + \varepsilon_z) + \tau_x \varepsilon_x. \]

Finally, by changing the origin \( \mathbf{p}_0 \) of the momentum basis, we eliminate two energies \( \varepsilon_{y,z} \). Discarding also the inconsequential energy \( \varepsilon_0 \) at \( \tau_0 \), we arrive at the final desired form

\[ \hat{H}(\mathbf{p}) = \tau_0 (v_{0x} p_x + v_{0y} p_y) + \tau_y v_{yx} p_x + \tau_z (v_{zx} p_x + v_{zy} p_y) + \tau_x \Delta \]  

(S2)
of the Hamiltonian, where we denoted $\varepsilon_x \equiv \Delta$. It is characterized by 6 real parameters: 5 velocities and 1 energy $\Delta$. The bulk spectrum of Eq. (S2) reads

$$
\varepsilon_{\pm}(p) = v_0 y p_y + v_0 x p_x \pm \sqrt{(v_{zy} p_y + v_{zx} p_x)^2 + (v_{yx} p_x)^2 + \Delta^2}. \tag{S3}
$$

Counting the degrees of freedom, we have used 6 available free parameters to represent the edge-state problem with the most general Hamiltonian (S1) with 11 substantial parameters and arbitrary edge orientation to that with the Hamiltonian (S2) with 6 parameters and $y = 0$ edge.

The simplest Hamiltonian

$$\hat{H}(p) \rightarrow v(\tau_y p_x + \tau_x p_y) + \tau_x \Delta, \tag{S4}$$

equivalent to Eq. (2) via an additional change of basis, is obtained from Eq. (S2) when $v_0 y, v_0 x, v_{zx} = 0$ and $v_{zy} = v_{xx} = v$.

### B. General boundary condition

We now derive the most general form of the BC for the Hamiltonian (S2). Mathematically, such BC is a single linear homogeneous relation between the two components $\psi_a, b(x, y = 0)$ of the wave function at the edge $y = 0$; without loss of generality, it can be written as

$$e^{i \frac{\phi}{2}} \sin \frac{\theta}{2} \psi_a(x, y = 0) - e^{-i \frac{\phi}{2}} \cos \frac{\theta}{2} \psi_b(x, y = 0) = 0, \tag{S5}$$

parameterized by two real angles $\theta$ and $\phi$.

The BC must only satisfy the fundamental constraint that the current perpendicular to the edge vanishes at the edge. For the Hamiltonian (S2), the operator of the current perpendicular to the $y = 0$ edge reads

$$\hat{j}_y = \partial_{p_y} \hat{H}(p_x, p_y) = \tau_x v_{zy} + \tau_0 v_0 y.$$  

It is given by the matrix at $p_y$ in Eq. (S2), which has conveniently been made diagonal.

Demanding that for any wave function satisfying Eq. (S5) the current $\hat{j}_y \psi(x, y = 0) = 0$ vanish, we obtain that the angle $\theta \equiv \theta_v \in (0; \pi)$ in Eq. (S5) is fixed by the velocity parameters of the bulk Hamiltonian as

$$\cos \theta_v = -\frac{v_0 y}{v_{zy}}, \tag{S6}$$

while the angle $\phi$ may be arbitrary$^2$.

And so, the most general form of the BC for the $y = 0$ edge for the most general linear Hamiltonian represented in the form (S2) reads

$$e^{i \frac{\phi}{2}} \sin \frac{\theta}{2} \psi_a(x, y = 0) - e^{-i \frac{\phi}{2}} \cos \frac{\theta}{2} \psi_b(x, y = 0) = 0. \tag{S7}$$

All unique forms of the BC are parameterized by the angle $\phi$ covering the full circle, similar to the angle $\theta$ in Eq. (3).

### C. Edge states and chiral and charge-conjugation symmetries

The edge states for the Hamiltonian (S2) and BC (S7) for the sample occupying the $y > 0$ half plane can be straightforwardly found. For every value of $\phi$ except $\pm \frac{\pi}{2}$, there exists one edge-state band

$$\mathcal{E}(p_x) = (v_{0x} + v_{zx} \cos \theta_v + v_{yx} \sin \theta_v \sin \phi) p_x + \Delta \sin \theta_v \cos \phi \tag{S8}$$

for any value of the gap $\Delta$, located at $p_x > p_x^m(\phi)$ for $\phi \in (-\frac{\pi}{2}, \frac{\pi}{2})$ and at $p_x < p_x^m(\phi)$ and for $\phi \in (\frac{\pi}{2}, \frac{3\pi}{2})$. Here,

$$p_x^m(\phi) = \frac{\Delta}{v_{yx}} \tan \phi, \quad \epsilon^m(\phi) = \frac{\Delta}{v_{yx} \cos \phi} \left[|v_{yx} \sin \theta_v + (v_{0x} + v_{zx} \cos \theta_v)| \sin \phi\right]$$

are the momentum and energy, at which the edge-state spectrum $\mathcal{E}(p_x)$ merges with the boundaries

$$\varepsilon_{+x}(p_x) = \min_{p_y} \varepsilon_{+}(p_x, p_y), \quad \varepsilon_{-x}(p_x) = \max_{p_y} \varepsilon_{-}(p_x, p_y)$$
of the continua of the bulk spectrum [Eq. (S3)], given by
\[ \varepsilon_{\pm x}(p_x) = (v_{0x} + v_{zx} \cos \theta_v)p_x \pm \sqrt{(v_{yx}p_x)^2 + \Delta^2 \sin \theta_v}. \] (S9)

Therefore, for the most general form of the linear model [Eqs. (S2) and (S7)], the edge-state structure in the vicinity of the TPT in a QAH system is nearly always (i.e., for all \( \phi \neq \pm \frac{\pi}{2} \)) extended beyond the minimal one required to satisfy the Chern numbers. As with the simplest Hamiltonian (2), below we analyze and explain this behavior in terms of chiral and charge-conjugation symmetries, also providing some additional details.

A bulk Hamiltonian satisfies chiral symmetry\(^3,4\), if there exists a unitary operation
\[ S[\hat{\psi}](r) = \hat{S}\psi(r) \] (S10)
on the wave function \( \hat{\psi}(r) = (\psi_a(r), \psi_b(r))^T \), where \( \hat{S} \) is a unitary matrix and \( r = (x, y) \) is a radius vector, under which the Hamiltonian changes its sign; in momentum space, for \( \hat{\psi}(p) = \int dr e^{-ipr}\hat{\psi}(r) \), this reads
\[ S[H](p) = \hat{S}H(p)\hat{S} = -\hat{H}(p). \] (S11)

We notice that the part
\[ \hat{H}_0(p) = \tau_y v_{yx}p_x + \tau_z (v_{zx}p_x + v_{zy}p_y) \] (S12)
of the Hamiltonian \( \hat{H}(p) \) [Eq. (S2)] (with \( v_{0x}, v_{0y}, \Delta = 0 \)) satisfies chiral symmetry with
\[ \hat{S} = \tau_x, \]
while the velocity \( \tau_0(v_{0x}p_x + v_{0y}p_y) \) and gap \( \tau_x\Delta \) terms break such chiral symmetry.

Similarly, a bulk Hamiltonian satisfies charge-conjugation symmetry\(^3,4\), if there exists an anti-unitary operation
\[ C[\hat{\psi}](r) = \hat{C}\psi^*(r) \] on the wave function, where \( \hat{C} \) is a unitary matrix and \( ^* \) denotes complex conjugation, under which the Hamiltonian changes its sign; in momentum space, this reads
\[ C[H](p) = \hat{C}\hat{H}^*(\mathbf{-p})\hat{C}^\dagger = -\hat{H}(p). \] (S13)

We notice that the whole Hamiltonian \( \hat{H}(p) \) [Eq. (S2)] satisfies charge conjugation symmetry with
\[ \hat{C} = \tau_z \]
and \( C^2 = +1 \).

Next, we analyze the BC (S7) in terms of symmetries. Chiral symmetry of the BC means that if a wave function \( \hat{\psi}(r) = (\psi_a(r), \psi_b(r))^T \) satisfies the BC, then the wave function \( \hat{S}[\hat{\psi}](r) = (\psi_a(r), \psi_b(r))^T \) transformed by the chiral symmetry operator (S10) also satisfies the same BC. Substituting \( \hat{S}[\hat{\psi}](r) \) into the BC (S7), we obtain
\[ e^{+i\frac{\phi}{2}}\sin \frac{\theta_v}{2}\psi_b(x, y = 0) - e^{-i\frac{\phi}{2}}\cos \frac{\theta_v}{2}\psi_a(x, y = 0) = 0. \]

This condition is identical to Eq. (S7) only if \( \theta_v = \frac{\pi}{2} \), i.e., \( v_{0y} = 0 \) [Eq. (S6)], and
\[ \phi = 0 \text{ or } \pi. \]
Therefore,
\[ \psi_a(x, y = 0) \mp \psi_b(x, y = 0) = 0, \] (S14)
respectively, are the only two chiral-symmetric forms of the BC (S7), possible only when \( v_{0y} = 0 \).

So, the chiral-symmetric Hamiltonian \( \hat{H}_0(p) \) [Eq. (S12)] with one of the chiral-symmetric BCs (S14) represents a 2D chiral-symmetric semimetal with an edge. Due to the well-defined winding number 1, such semimetal exhibits flat edge-state bands that are topologically protected by chiral symmetry\(^4\). Indeed, it follows from Eq. (S8) that in this case the edge-state band \( E(p_x) \equiv 0 \) is flat and located at \( p_x > 0 \) for \( \phi = 0 \) and at \( p_x < 0 \) for \( \phi = \pi \).
The remaining gap $\tau_x \Delta$ and velocity $\tau_0(v_{0x} p_x + v_{0y} p_y)$ terms in the bulk Hamiltonian $\hat{H}(\mathbf{p})$ [Eq. (S2)] and the deviations of the angle $\phi$ of the BC (S7) from 0 or $\pi$ break chiral symmetry. Nonetheless, the edge-state band (S8) persist. At the TPT $\Delta = 0$, when the system is gapless, the edge-state band exists for any values of $v_{0x}$ and $v_{0y}$ and any value of $\phi \neq \pm \frac{\pi}{2}$: the velocity

$$V(\phi) = \partial_{p_x} \mathcal{E}(p_x) = v_{0x} + v_{xz} \cos \theta_v + v_{yz} \sin \theta_v \sin \phi$$

(S15)
of the edge-state band (S8) is always between the velocities

$$v_{\pm x} = \partial_{p_x} \mathcal{E}(p_x)|_{\Delta=0} = v_{0x} + v_{xz} \cos \theta_v \pm |v_{yz}| \sin \theta_v$$

(S16)
of the dispersion relations (S9) determining the boundaries of the continua of the bulk spectrum, $V(\phi) \in [v_{-x}, v_{+x}]$, reaching them only at $\phi = \pm \frac{\pi}{2}$, as shown in Fig. S1.

The values $\phi = \pm \frac{\pi}{2}$ are actually special symmetry-wise. As with chiral symmetry, a BC is charge-conjugation-symmetric if the transformed wave function $\mathcal{C}[\hat{\psi}](\mathbf{r}) = (\psi^*_a(\mathbf{r}), -\psi^*_b(\mathbf{r}))^T$ also satisfies the same BC. Substituting $\mathcal{C}[\hat{\psi}](\mathbf{r})$ into the BC (S7), we obtain

$$e^{-i \frac{\theta}{2}} \psi_a(x, y = 0) + e^{i \frac{\theta}{2}} \psi_b(x, y = 0) = 0,$$

which is identical to Eq. (S7) only if

$$\phi = \pm \frac{\pi}{2}.$$

Therefore, $e^{i \frac{\theta}{2}} \psi_a(x, y = 0) - e^{-i \frac{\theta}{2}} \psi_b(x, y = 0) = 0$, respectively, are the only two charge-conjugation-symmetric forms of the BC (S7). Thus, as with the simplest Hamiltonian (2)$^5$, for the most general form (S2) of the linear Hamiltonian, the only cases of the general BC (S7), in which the edge-state band at the TPT $\Delta = 0$ induced by chiral symmetry is absent, are the ones that have charge-conjugation symmetry. The intervals $\phi \in (-\frac{\pi}{2}, \frac{\pi}{2})$ and $\phi \in (\frac{\pi}{2}, \frac{3\pi}{2})$, separated by the points $\phi = \pm \frac{\pi}{2}$, are the stability regions of the chiral-symmetric cases $\phi = 0, \pi$.

The above-described edge-state band induced by chiral symmetry at the TPT is not required by QH topology. Therefore, it represents the extension of the edge-state structure at TPT and also in gapped TnT and TT phases: a finite gap modifies this edge-state band only in the momentum region dominated by the gap, as explained in the Main Text.

We have thus demonstrated with the most general form of the linear model [Eqs. (S2) and (S7)] that the main claim of the paper is completely general and not specific to the simplest form (1) of the bulk Hamiltonian considered in the Main Text: the edge-state structure in the vicinity of the TPT in a QAH system is nearly always significantly extended beyond the minimal one required to satisfy the Chern numbers.
II. QUADRATIC MODEL OF A QUANTUM ANOMALOUS HALL SYSTEM

Here, we present in more detail the properties of the quadratic model described by Eqs. (6) and (7).

A. Boundary condition for the linear model

Here, we derive the BC of the form (3) for the linear model (2) that asymptotically describes the quadratic model with the Hamiltonian (6) and BCs (7) in the vicinity of its TPT $\Delta = 0$. The systematic procedure is as follows. Let us first find the general solution to the Schrödinger equation

$$\hat{H}_2(p_x, \hat{p}_y)\hat{\psi}(y) = \epsilon \hat{\psi}(y)$$

right at the TPT $\Delta = 0$ for momentum $p_x = 0$ and energy $\epsilon = 0$ exactly at the node that contains no contributions growing into the bulk. We obtain

$$\hat{\psi}(y) = \begin{pmatrix} \psi_a \\ \psi_b \end{pmatrix} + Be^{-\kappa y} \begin{pmatrix} \sqrt{\beta_b} \\ \sqrt{\beta_a} \end{pmatrix},$$

with the momentum scale

$$\kappa = \frac{v}{\sqrt{\beta_a \beta_b}} \quad \text{(S17)}$$

and three independent constant coefficients $\psi_{a,b}$ and $B$. Applying the BCs (7) to it and excluding $B$, we arrive at the constraint

$$\sqrt{\beta_a} \psi_a - \sqrt{\beta_b} \psi_b = 0. \quad \text{(S18)}$$

The quantity $\kappa$ defines the validity scale of the low-energy model with the linear Hamiltonian (2): the momentum scales of interest $p_x, \epsilon/v, p_\Delta \ll \kappa$ must be small. Accordingly, the wave function $\hat{\psi}(r) = (\psi_a(r), \psi_b(r))^T$ of the linear Hamiltonian (2) must vary slowly at the spatial scale $1/\kappa$. To the leading order, the relation (S18) will still apply to the components $\psi_{a,b} \rightarrow \psi_{a,b}(x, y = 0)$ of such wave function at the edge. Thus, the relation (S18) represent the BC of the form (3) with the angle $\theta$ determined by the ratio of the curvatures as expressed in Eq. (8).

B. Charge-conjugation symmetry

The quadratic Hamiltonian (6) satisfies change-conjugation symmetry [Eq. (S13)] with $\hat{C} = \tau_x$ only if $\beta_a = \beta_b$. Its hard-wall BCs (7) also satisfy this symmetry. Only in this case the minimal edge-state structure required to satisfy the Chern numbers is realized, shown in Fig. 1(d),(e),(f).

C. Extension of the edge-state structure

Here, we discuss in more detail the effect of the extension of the edge-state structure beyond the minimal one required to satisfy the Chern numbers in the quadratic model of a QAH system described by Eqs. (6) and (7).

The model is described by four parameters, the gap $\Delta$, velocity $v$, and curvatures $\beta_{a,b}$. We observe that instead of $\beta_{a,b}$ it is more physically insightful to consider the combinations

$$\beta = \sqrt{\beta_a \beta_b}, \ t = \sqrt{\frac{\beta_a}{\beta_b}} \quad \text{(S19)}$$

as independent parameters, in terms of which

$$\beta_a = \beta t, \ \beta_b = \beta \frac{1}{t}.$$ 

This way, the geometric mean $\beta$ sets the overall momentum $\kappa$ [Eq. (S17)] and energy

$$\epsilon = v \kappa = \frac{v^2}{\beta} \quad \text{(S20)}$$
FIG. S2: (a) The dependence on the dimensionless gap $\tilde{\Delta} = \Delta / \varepsilon$ of the dimensionless energies $\tilde{\varepsilon}^{m,\pm}(\tilde{\Delta}, t) = \varepsilon^{m,\pm}/\varepsilon$ [Eq. (S22), red and green] of the merging points of the edge-state band in the quadratic model [Eqs. (6) and (7)] of a QAH system (also describing one block of the BHZ model of a QSH system). The grey-shaded regions denote the continua of the bulk states of the conduction and valence bands. (b)-(e) The samples of the edge-state spectra (blue) at various values of $\tilde{\Delta}$, indicated in (a), describing different regimes. The graphs are plotted for the value $t = 2.31$ [Eq. (S19)] that corresponds to the parameters (Tab. S1) estimated in Ref. 6 for a HgTe quantum well at the topological phase transition. For presentation purposes, we used the plot aspect ratios different from 1, which can be deduced from the provided tick values.

FIG. S3: Same as in Fig. S2 for the value $t = 1.26$ [Eq. (S19)] that corresponds to the parameters (Tab. S1) estimated in Ref. 6 for an InAs quantum well at the topological phase transition.

scales of the quadratic model, which, in particular, define the range of validity of the linear model, as explained in Sec. II.A. The dimensionless parameter $t$, on the other hand, fully characterizes the asymptotic edge-state structure [Eq. (4)] in the vicinity of the TPT through Eq. (8) for the parameter of the BC (3) of the linear model. This "asymmetry" parameter $t$ describes the deviation from the charge-conjugation symmetry point $t = 1$, at which the extension of the edge-state structure is absent. The more $t$ deviates from 1, the closer one is to the chiral-symmetric case and the flatter the edge-state band (4) is. The quadratic model is thus fully characterized by two dimensionless
parameters, $t$ and $\bar{\Delta} = \Delta/\varepsilon$, while the two dimensional parameters, say, $\kappa$ and $\varepsilon$, set the natural units of measurement. When measured in the units of $\kappa$ and $\varepsilon$, the momenta $p^{m\pm}$ [Eq. (9)] of the merging points of the edge-state band and their energies

$$e^{m\pm} = \frac{1}{(\beta_a + \beta_b)^2} \left[ -\Delta (\beta_a^2 - \beta_b^2) + v^2 (\beta_a - \beta_b) \left( -1 \pm \sqrt{1 - 8 \Delta \beta_a \beta_b (\beta_a + \beta_b) / v^2 (\beta_a - \beta_b)^2} \right) \right]$$

are presentable as dimensionless functions

$$p^{m\pm}_x (\Delta, t) = \frac{p^{m\pm}_x}{\kappa} = \frac{1}{2} \left( t - \frac{1}{t} \right) \left( -1 \pm \sqrt{1 - \frac{\Delta}{\Delta^*}} \right),$$

$$e^{m\pm} (\Delta, t) = \frac{e^{m\pm}}{\varepsilon} = -\frac{\Delta (t - \frac{1}{t})}{t + \frac{1}{t}} + \frac{t - \frac{1}{t}}{(t + \frac{1}{t})^2} \left( -1 \pm \sqrt{1 - \frac{\Delta}{\Delta^*}} \right)$$

of the dimensionless gap $\bar{\Delta}$ and parameter $t$. Here,

$$\Delta^* = \frac{v^2 (\beta_a - \beta_b)^2}{8 \beta_a \beta_b (\beta_a + \beta_b)} = \varepsilon \Delta^*, \quad \bar{\Delta}^* = \frac{1}{8} \left( t - \frac{1}{t} \right)^2$$

is the critical value of the gap in the TT phase, at which the edge-state band disappears. The edge-state band exists for all $\Delta < \Delta^*$, i.e., in the TnT phase for $\Delta < 0$ (where, in the vicinity of the TPT, $|\Delta| \ll \varepsilon$, it extends beyond the gap region), at the TPT $\Delta = 0$, and in the TT phase for $0 < \Delta < \Delta^*$ up to this critical value. As explained in the Main Text, this behavior constitutes the extension of the edge-state structure beyond the minimal one required to satisfy the Chern numbers. The critical gap $\Delta^*$ characterizes the magnitude of the extension effect and is determined by both the deviation of $t$ from 1 (the case of charge-conjugation symmetry) and the energy scale $\varepsilon$ [Eq. (S20)].

In Figs. S2 and S3, we plot the dependence of the dimensionless energies $e^{m\pm} (\Delta, t)$ [Eq. (S22)] of the merging points on dimensionless gap $\bar{\Delta}$, for two values of $t$ that correspond to the sets of parameters, presented in Tab. S1, of the BHZ model that have been estimated in Ref. 6 for QSH systems realized in quantum wells. We use the parameters for the cases that are very close to the TPT, with thicknesses $d = 6.1$nm and 9.0nm for HgTe/CdTe and InAs/GaSb/AlSb quantum wells, respectively. For HgTe, Fig. S2, both the deviation of the asymmetry parameter $t = 2.31$ from 1 and the energy scale $\varepsilon = 354$meV are quite large, giving an experimentally appreciable critical value $\Delta^* = 57$meV and implying quite a pronounced extension effect. For InAs, on the other hand, Fig. S3, the asymmetry parameter $t = 1.26$ is close to 1, i.e., the system is much closer to the case of charge-conjugation symmetry, and the energy scale $\varepsilon = 5.04$meV is small due to the much smaller velocity $v$ compared to the HgTe case; as a result, the extension effect is weak, with an experimentally small critical value $\Delta^* = 0.070$meV.

In Figs. S2 and S3, the grey-shaded regions denote the continua of the conduction- and valence-band states

$$\varepsilon_{\pm} (p) = \frac{1}{2} (\beta_a - \beta_b) p^2 \pm \sqrt{[\Delta + \frac{1}{2} (\beta_a + \beta_b) p^2]^2 + (vp)^2}, \quad p^2 = p_x^2 + p_y^2,$$

of $\hat{H}_2 (p)$ [Eq. (6)], respectively, as all momenta $p$ are spanned. These energy regions are bounded by the minimum

$$\varepsilon_{+0} = \min_p \varepsilon_{+} (p)$$

of the conduction band and maximum

$$\varepsilon_{-0} = \max_p \varepsilon_{-} (p)$$

of the valence band, given by

$$\varepsilon_{\pm 0} = \begin{cases} 
\frac{1}{(\beta_a + \beta_b)^2} \left[ -\Delta (\beta_a^2 - \beta_b^2) - v^2 (\beta_a - \beta_b) \pm 2v \sqrt{\beta_a \beta_b [-2\Delta (\beta_a + \beta_b) - v^2]} \right], \quad \Delta < \Delta_{\pm 0}, \\
\pm |\Delta|, \quad \Delta_{\pm 0} < \Delta,
\end{cases}$$

$$\Delta_{+0} = -\frac{v^2}{2\beta_b}, \quad \Delta_{-0} = -\frac{v^2}{2\beta_a}.$$
HgTe, $d = 6.1$ nm & 378 & 931 & 175 & 404 & 2.31 & 354 & 57 \\ InAs, $d = 9.0$ nm & 62 & 963 & 603 & 762 & 1.26 & 5.04 & 0.070 

| TABLE S1: Parameters of the BHZ model estimated in Ref. 6 for HgTe and InAs quantum wells at the topological phase transition; $d$ is the thickness of the active layer. Similar values of parameters for a HgTe quantum well were estimated in Ref. 7. |

In the dimensionless units,

$$
\bar{\varepsilon}_{\pm 0}(\bar{\Delta}, t) = \frac{\varepsilon_{\pm 0}}{\bar{\varepsilon}} = \begin{cases} 
-\frac{\Delta}{t} \frac{1}{t+\frac{1}{2}} - \frac{1}{t+\frac{1}{2}} - \frac{2}{t+\frac{1}{2}} \sqrt{-2\Delta(t+\frac{1}{2}) - 1}, & \Delta < \Delta_{\pm 0}, \\
\Delta_{\pm 0} = \frac{\Delta_{\pm 0}}{\varepsilon} = -\frac{1}{2t}.
\end{cases}
$$

At $\Delta_{\pm 0} < \Delta$, the dispersion relation $\varepsilon_{\pm}(p)$ is monotonic in $p$ and its absolute minimum/maximum (for $\pm$, respectively) $\varepsilon_{\pm}(0) = \pm |\Delta|$ is reached at $p = 0$. However, at $\Delta < \Delta_{\pm 0}$, $\varepsilon_{\pm}(p)$ becomes nonmonotonic ("mexican-hat" regime) and its absolute minimum/maximum is reached at a finite value of $p$. We point out that the latter regime occurs at large enough negative $\Delta < \Delta_{\pm 0}$, i.e., away from the TPT, where the extension effect we predict is not present anymore. The formulas for the edge-state dispersion relation [Eqs. (4) and (8)] and merging points [Eqs. (9) and (S21)] are valid in all regimes of $\Delta$. In Fig. S2 for HgTe, the transition point $\Delta_{-0}$ is within the plot range, while $\Delta_{+0}$ is not; in Fig. S3 for InAs, both $\Delta_{\pm 0}$ are outside of the plot range.

For the BHZ model of a QSH system, the model (6) and (7) of the QAH system represents one Kramers block, and the full spectrum is obtained by adding the counterparts obtained by time reversal.

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1. To avoid confusion, we point out that, in general, the labels $x, y, z$ of the Pauli matrices have no physical meaning of and no relation to the directions in real and momentum spaces.
2. Note that for a single node in the whole Brillouin zone described by Eq. (S2), the system with an edge can be defined only if $|v_{0y}| < |v_{zy}|$.
3. S. Ryu, A. Schnyder, A. Furusaki, and A. Ludwig, New J. Phys. 12, 065010 (2010).
4. C.-K. Chiu, J. C.Y. Teo, A. P. Schnyder, and S. Ryu, Rev. Mod. Phys. 88, 035005 (2016).
5. For the simplest Hamiltonian in the form (2) used in the Main Text, $\hat{C} = \tau_z$ and the BC (3) is charge-conjugation-symmetric at $\theta = \pm \frac{\pi}{2}$.
6. Tab. 1 on p. 64 and Tab. 2 on p. 65 in C. Liu and S.-C. Zhang, Chapter "Models and Materials for Topological Insulators" in "Topological insulators", edited by M. Franz and L. Molenkamp.
7. D. G. Rothe, R. W. Reinthaler, C.-X. Liu, L. W. Molenkamp, S.-C. Zhang, and E. M. Hankiewicz, New J. Phys. 12, 065012 (2010).