Anomalous bulk-boundary correspondence in dimerized topological insulators

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The bulk-boundary correspondence is a generic feature of topological states of matter, reflecting the intrinsic relation between topological bulk and boundary states. For example, robust edge states propagate along the edges and corner states gather at corners in the two-dimensional first-order and second-order topological insulators, respectively. Here, we report two kinds of topological states hosting anomalous bulk-boundary correspondence in the extended two-dimensional dimerized lattice with staggered flux threading. At 1−filling, we observe isolated corner states with no fractional charge as well as metallic near-edge states in the C = 2 Chern insulator states. At 1 filling, we find a C = 0 topologically nontrivial state, where the robust edge states are well localized along edges but bypass corners. These robust topological insulating states significantly differ from both conventional Chern insulators and usual high-order topological insulators.

Introduction.—The bulk-boundary correspondence in topological states reveals the intrinsic relationship between topological invariants and boundary states [1, 2]. For instance, the soliton excitation with a e/2 fractional charge in Su-Schrieffer-Heeger (SSH) model is the prototype bulk-boundary correspondence in one dimension [3, 4]. In two-dimensional (2D) topologically non-trivial states of matter, topologically protected boundary states propagating along the edges are robust against defects and cannot diffuse into the bulk or only gather at corners. As a representative, Chern insulators (CIs) first proposed in the honeycomb lattice by staggered flux threading[5] and later experimentally realized in ultracold fermion system [6] and magnetic topological insulators [7] host the gapped bulk bands and the gapless chiral edge modes. Such bulk-edge correspondence is universal in all CIs established on various crystal lattice models, such as the checkerboard-lattice model [8, 9], the kagome-lattice model [10, 11], and other exotic lattice models [12–18]. Even in aperiodic systems, for example the quasicrystalline CI on the Diir’s tiling proposed recently [19], bulk-edge correspondence remains applicable.

In contrast, in higher-order topological insulators (HOTIs), the conventional bulk-edge correspondence no longer applies [20–31]. HOTIs belong to a special class of topological states, hosting (d − f)-dimensional boundary states where d labels dimensions of the bulk and f the order of HOTIs. Some 2D HOTIs are characterized by the nested Wilson loop [20, 21], reflecting the topological property of Wannier bands. As a sequence, gapped edge states and topologically protected corner states are observed, together with fractional charges at corners. There are also some unconventionally topological states hosting special bulk-boundary correspondence.

Zero Chern number (i.e., C=0), but with topologically protected edge states had been reported in the half-filled dimerized Hofstadter model [32] and the quarter-filled 2D SSH model [33]. So far, the boundary states observed in the 2D topological insulators are either edge-like or corner-like. Whether there co-exist both the isolated corner and gapless edge states in the same topological boundary state remains unclear.

In this letter, we report two kinds of topologically insulating states hosting anomalous bulk-boundary correspondence in a 2D dimerized square lattice model with

![Schematic structure of an extended SSH model on a square lattice. The lattice vectors are \( \vec{a}_1 \), \( \vec{a}_2 \) and within the unit cell, there are four atoms. Black and purple bonds represent the intracellular (the dashed square) NN \( (w) \) and NNN \( (w') \) hoppings, respectively, and red bonds are the intercellular hoppings \( (v) \). The staggered fluxes are \( \phi \) in the intercellular square, 0 for the fully dimerized square and \(-2\phi\) in the both remaining squares, respectively. The adopted gauge is explicitly displayed by arrows, with an additional phase factor \( \pm\phi \) for part of the NN hopping process.](image-url)
staggered flux threading. At 1/2-filling, we find a $C = 2$ Chern insulator state. In sharp contrast to the previous reported CIs, the boundary states both gather around the corners and extend into quasi-edges, leading to isolated corner states and metallic near-edge state. This special bulk-boundary correspondence is well identified by Wannier bands, where a significant shift of Wannier bands is observed. We argue that the anomaly originates from the existence of 1D SSH-like domain walls at corners, which isolate the corner states and push the edge states into the quasi-edge. On the other hand, a zero-Chern number topological insulator state emerges at 1/4-filling. The boundary states bypass the corners and localize along the edges robustly. Our findings shed light on novel bulk-boundary correspondences in topological insulators and offer opportunities to search for more anomalous topological states.

Model.— Our starting model is an extended version of the 2D SSH model[3, 4] with staggered flux threading the plaquettes as illustrated in Fig. 1. The Hamiltonian is given by

$$H = w \sum_{\langle r,r' \rangle} \left[ c_r^\dagger c_r \exp (i\phi_{rr'}) + \text{H.c.} \right] + w' \sum_{\langle \langle r,r' \rangle \rangle} \left[ c_r^\dagger c_r + \text{H.c.} \right] + v \sum_{\langle r,r' \rangle} \left[ c_r^\dagger c_{r'} + \text{H.c.} \right] \quad (1)$$

where $c_r^\dagger (c_r)$ is the creation (annihilation) operator of a spinless electron at site $r$. $\langle \cdots \rangle$ and $\langle\langle \cdots \rangle\rangle$ denote the intracellular nearest-neighbor (NN), and the next-nearest-neighbor (N2N) hopping process with the hopping integral $w$, and $w'$, respectively. $\langle \cdots \rangle'$ denotes the intercellular NN hopping with the amplitude $v$. $\phi_{rr'} = \pm \phi$ is the phase factor in the intracellular NN hopping process with sign denoted by the arrow. Numerically, we set the intracellular NN hopping integral $w$ as unit, $w' = 0.75$, and $\phi = \pi - 0.25\pi$ unless specified. The present model reduces to the 2D SSH model in the absence of the flux and NNN hopping, where a Zak phase accompanied by the fractional wave polarization with vanishing Berry curvature in the first Brillouin zone is revealed [33]. Similar dimerized 2D lattice model with $\pi$ flux threading hosts a HOTI in which the robust corner states with a fractional corner charge $e/2$ emerge due to the quantized quadrupole moments [20, 21].

We show the energy bands evolution on the intercellular hopping $v$ on the cylinder geometry (shown in Fig. 2). There are four bands in our model. A significant band gap between the upper two and lower two bands emerges with two chiral edge modes, suggesting a CI with $C = 2$ at half-filling. On the other hand, the band gap between the two lowest bands evolves from the indirect gap to the direct gap with increasing $v$, indicating a metallic to insulating phase transition.

$C = 2$ Chern insulator states at 1/2-filling.— The topological property at 1/2-filling can be identified by the Chern number $C = \sum_{k_r < E_F} C_n$ on the torus geometry. Here, $E_F$ is the Fermi energy and $C_n$ is the subband Chern number calculated by integrating the Berry curvature over the first Brillouin zone [11, 34, 35]. Numerical results show that the model hosts phase transitions from a trivial state with $C = 0$ to a topologically nontrivial state with $C = 2$ at the critical point $v = 0.75$, which can also be identified with the aid of band gap $\Delta$ [Fig. 3(a)]. This Chern insulator state agrees with the spectrum on the cylinder geometry, where two branches of chiral edge states appear in the band gap. In order to present the topological features in the open system more accurately, we further compute the real-space Chern number based on the Kitaev formula [35, 36]. In Fig. 3 (a) (red line), we present the real-space Chern number with a selected Fermi energy at the 800th energy level in a $20 \times 20 \times 4$ square lattice [Fig. 3 (b)]. The real-space Chern number is near two when $v > 0.80$, which is slightly larger than the critical value of 0.75 on the torus geometry due to the finite-size effect.

To account the topological properties of the boundary states, we divide the lattice with open boundary into four parts—the corners, the edges (excluding corners), the quasi-edge, and the bulk [as illustrated in Fig. 3 (b)]. Spatial distributions of the boundary states are shown in Fig. 3 (d)-(e). Interestingly, the corner states are gradually enhanced while the edge states are weakened with increasing $v$ [35]. At a stronger dimerized potential ($v > 2.2$), the edge states slightly diffuse into the bulk, leaving the edges empty and the corner states isolated—we dub them as the near-edge states. These features are in sharp contrast to the well edge-localized boundary states in the conventional CIs [35], suggesting anomalous topological features of the boundary states at half-filling. We define the ratio of corner density as $\rho = |\phi_{\text{cor}}^n|^2 / |\phi_{\text{bd}}|^2$ to measure the proportion of the corner states in the boundary states (including corners and edges), where $|\phi_{\text{cor}}^n|^2$ and $|\phi_{\text{bd}}|^2$ denotes the corner, and the boundary density of the $n$-th state. The ratio $\rho$ of the
800th state enhances with the increasing $\nu$ [Fig. 3 (f)]. At strong dimerization limit, the ratio nearly equals to 1.0, which suggests the boundary states are fully gapped out. In fact, the in-gap states host similar tendency as shown in the average ratio of the corner density from the 780th to the 820th in-gap states. The coexistence of corner and near-edge states is robust against the strong intercellular hopping in the present topological state, for example, $v = 20$ and $v = 50$ [35]. These special boundary states are also robust against defects and lattice sizes [35]. We emphasize that no fractional charge at corners emerges even at strong dimerization limit (details see Ref. [35]), suggesting the CI rather than the HOTI nature [20, 21] of the present topological state.

In some 2D HOTIs, topological properties are well characterized by the topological invariant—nested Wilson loop [20, 21], where the gapped Wannier bands are discovered. On the contrary, Wannier bands are gapless in the conventional CIs [21, 31], consisting with gapless edge states. Here, we further study Wannier bands to identify the present CI state. The Wannier spectra are shown in Fig. 4 (a). The gapless Wannier bands in our model manifest the CI nature of the present topological state. Wannier centers crossing a reference line twice further confirm the $C = 2$ Chern insulator state. Such features are in sharp contrast to the gapped Wannier bands in a HOTI [Fig. 4 (b)] [20, 21]. On the other hand, unlike the exact value $\nu_x = \pm 1/2$ at $k_y = \pm \pi$ in the conventional CI states [such as the Haldane model[5, 37] and the checkerboard model[9] in Fig. 4 (b)], a significant Wannier band shifting is observed in our present model. This agrees well with the special features of the isolated corner states and the near-edge states, manifesting a special bulk-boundary correspondence.

In our present model, there exists 1D SSH-like domain walls at corners [3, 4]. At a weak dimerization, the domain wall remains trivial and the system exhibits a conventional CI nature with robust edge states [35]. On the contrary, at a strong dimerization, the nontrivial domain walls yield the gapped boundary states and isolated corner states but without fractional charge. Concomitantly, the gapped boundary pushes the gapless edge states inherited from the CI nature into quasi-edges, i.e., the chiral near-edge states. Moreover, different from the simple SSH model, intracellular hopping contains the NNN processes and the additional phase factors, which strengthens the effective intracellular hopping potential.

$C = 0$ topological state at 1/4-filling.—We now study the topological properties of the proposed model at 1/4-filling. By tuning intercellular hopping potential, chiral and helical-like edge states emerge (in Fig. 2), which suggests the appearance of various topological states.
We analyze their Wannier centers on torus geometry to identify these topological states [in Fig. 5 (a)]. In case of weak intercellular hopping $v < 0.75$, the Wannier bands show the typically normal insulating feature, i.e., $\nu_{x}(0) = \nu_{x}(\pi) = \nu_{x}(2\pi) \equiv 0$, as well the near zero value for other momentum. When $v \in (0.75, 2.2)$, a CI-like feature of the gapless Wannier band with $\nu_{x}(0) = 0.5$, $\nu_{x}(\pi) = 0$, and $\nu_{x}(2\pi) = -0.5$ emerges in the intermediate $v$ [35]. However, due to the indirect band gap between the lowest two bands shown in Fig. 2 (a), the present state is a metallic state.

Further increasing $v > 2.2$, the reopening band gap (in Fig. 2), together with specific Wannier centers indicate the emergence of another topological state [Fig. 5 (a)]. It should be reminded that there are two isolated edge modes in the band gap propagating reversely along the open boundaries [Fig. 2 (c)]. The topological state at $1/4$-filling is a zero-Chern number topological state, which is similar to the previously reported zero Berry curvature topological state in 2D SSH model [33]. On account of our model with inversion symmetry, topology of energy band can be further confirmed by the 2D Zak phase based on the parities at high symmetric points [32, 33, 35, 38, 39], which are marked as ±π displayed in Fig. 5 (b). We obtain the polarization $p = (1/2, 1/2)$, which is in accordance with the results of Wannier centers [shown in Fig. 5 (a)].

Spatial distribution of boundary state is presented in Fig. 5 (c). The boundary state is well localized along the edges but bypasses the corners, leaving the missing of corner states, which manifests an anomalous bulk-boundary correspondence. This topological state is contrary to the conventional topological states, in which both the edge and corner states exist. On the other hand, it also differs from the 2D HOTI states, where only corner states emerge. We also present phase diagram by tuning intercellular hopping $v$ and staggered flux $\phi$ [Fig. 5 (d)], which contains the normal insulator, the metal and the zero-Chern number topological phases. We notice there are no CI phase, because the present parameters are not able to absolutely open the band gap at $1/4$-filling and finally lead to a metal phase with CI-like features [Fig. 5 (d)].

**Summary and discussion.**—We have proposed two unconventional topological insulator states realized in the dimerized square lattice model with staggered flux threading. At half-filling, the $C = 2$ CI state, identified by the Chern number and the gapless Wannier bands, hosts an anomalous bulk-boundary correspondence—the coexistence of the isolated corner states and the near-edge states. We argue the anomaly comes from the existence of 1D SSH-like domain wall. At quarter-filling, we find another topological insulator state with $C = 0$. The boundary state is localized along the edges but in the absence of the corner state. The bulk-boundary correspondence reported here is in sharp contrast to that in the conventional topological insulators and the HOTIs. Our findings may add a new insight into the bulk-boundary correspondence in topological insulators, and offer opportunities to search exotic topological states.

Experimentally, a very promising approach to realize the dimerized quantum Hall states is the ultracold atomic
system, in which the Hofstadter model [40] and the Hal- 
dane model [6] had been realized. Recently, 2D dimerized 
lattices hosting HOTIs have been theoretically discussed 
and experimentally observed in phononic and electrical-
circuit systems [20, 29, 41–44], and CI states have been 
realized in electrical-circuit systems [45]. Hence, based on 
those potential ways to construct the dimerized lattices 
and simulate CI states, it would be natural to make ex-
perimental observation of more exotic topological states 
in various artificial microstructures. The observation of 
CI state in a multilayer graphene moiré superlattice [46– 
48] also creates a possible route to explore our present 
topological states.

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[1] M. Z. Hasan and C. L. Kane, Rev. Mod. Phys. 82, 3045 (2010).
[2] X.-L. Qi and S.-C. Zhang, Rev. Mod. Phys. 83, 1057 (2011).
[3] W. P. Su, J. R. Schrieffer, and A. J. Heeger, Phys. Rev. Lett. 42, 1698 (1979).
[4] W. P. Su, J. R. Schrieffer, and A. J. Heeger, Phys. Rev. B 22, 2099 (1980).
[5] F. D. M. Haldane, Phys. Rev. Lett. 61, 1955 (1988).
[6] G. Jotzu, M. Messer, R. Desbuquois, M. Lebrat, T. Uehlinger, D. Greif, and T. Esslinger, 
Nature 515, 237 EP (2014).
[7] C.-Z. Chang, J. Zhang, X. Feng, J. Shen, Z. Zhang, M. Guo, K. Li, Y. Ou, P. Wei, L.-L. Wang, Z.-Q. Ji, 
Y. Feng, S. Ji, X. Chen, J. Jia, X. Dai, Z. Fang, S.-C. Zhang, K. He, Y. Wang, L. Lu, X.-C. Ma, and Q.-K. Xue, 
Science 340, 167 (2013).
[8] V. M. Yakovenko, Phys. Rev. Lett. 65, 251 (1990).
[9] K. Sun, Z. Gu, H. Katsura, and S. Das Sarma, Phys. Rev. Lett. 106, 236803 (2011).
[10] H.-M. Guo and M. Franz, Phys. Rev. B 80, 113102 (2009).
[11] E. Tang, J.-W. Mei, and X.-G. Wen, Phys. Rev. Lett. 106, 236802 (2011).
[12] X.-L. Qi, Y.-S. Wu, and S.-C. Zhang, Phys. Rev. B 74, 085308 (2006).
[13] C. Weeks and M. Franz, Phys. Rev. B 82, 085310 (2010).
[14] H. Yao and S. A. Kivelson, Phys. Rev. Lett. 99, 247203 (2007).
[15] A. Rüegg, J. Wen, and G. A. Fiete, Phys. Rev. B 81, 205115 (2010).
[16] M. Kargarian and G. A. Fiete, Phys. Rev. B 82, 085106 (2010).
[17] X. Hu, M. Kargarian, and G. A. Fiete, Phys. Rev. B 84, 155116 (2011).
[18] Y.-F. Wang, H. Yao, C.-D. Gong, and D. N. Sheng, Phys. Rev. B 86, 201101 (2012).
[19] A.-L. He, L.-R. Ding, Y. Zhou, Y.-F. Wang, and C.-D. Gong, Phys. Rev. B 100, 214109 (2019).
[20] W. A. Benalcazar, B. A. Bernevig, and T. L. Hughes, Science 357, 61 (2017).
[21] W. A. Benalcazar, B. A. Bernevig, and T. L. Hughes, Phys. Rev. B 96, 245115 (2017).
[22] Z. Song, Z. Fang, and C. Fang, Phys. Rev. Lett. 119, 246402 (2017).
[23] J. Langbehn, Y. Peng, L. Trifunovic, F. von Oppen, and P. W. Brouwer, Phys. Rev. Lett. 119, 246401 (2017).
[24] F. Schindler, A. M. Cook, M. G. Vergniory, Z. Wang, S. S. P. Parkin, B. A. Bernevig, and T. Neupert, Science Advances 4 (2018).
[25] M. Ezawa, Phys. Rev. B 98, 045125 (2018).
[26] S. Franco, J. van den Brink, and I. C. Fulga, Phys. Rev. B 98, 011114 (2018).
[27] M. Ezawa, Phys. Rev. Lett. 120, 026801 (2018).
[28] L. Trifunovic and P. W. Brouwer, Phys. Rev. X 9, 011012 (2019).
[29] R. Chen, C.-Z. Chen, J.-H. Gao, B. Zhou, and D.-H. Xu, Phys. Rev. Lett. 124, 036803 (2020).
[30] E. Lee, A. Furusaki, and B.-J. Yang, Phys. Rev. B 101, 241109 (2020).
[31] A.-L. He, Y.-F. Wang, and H. Yao, (unpublished).
[32] A. Lau, C. Ortix, and J. van den Brink, Phys. Rev. Lett. 115, 216805 (2015).
[33] F. Liu and K. Wakabayashi, Phys. Rev. Lett. 118, 076803 (2017).
[34] D. J. Thouless, M. Kohmoto, M. P. Nightingale, and M. den Nijs, Phys. Rev. Lett. 49, 405 (1982).
[35] See Supplemental Material for more details about the topological invariants, characterization of these topological states, and the robustness of the topological states, etc.
[36] A. Kitaev, Annals of Physics 321, 2 (2006).
[37] Q. Qing, C. Wang, W. Luo, A. L. He, and Y. F. Wang, J Phys Condens Matter 30, 355502 (2018).
[38] T. L. Hughes, E. Prodan, and B. A. Bernevig, Phys. Rev. B 83, 245132 (2011).
[39] C. Fang, M. J. Gilbert, and B. A. Bernevig, Phys. Rev. B 86, 115112 (2012).
[40] M. Aidelsburger, M. Atala, M. Lohse, J. T. Barreiro, B. Paredes, and I. Bloch, Phys. Rev. Lett. 111, 185301 (2013).
[41] M. Serra-Garcia, V. Peri, R. Süssstrunk, O. R. Bilal, T. Larsen, L. G. Villanueva, and S. D. Huber, Nature 555, 342 (2018).
[42] C. W. Peterson, W. A. Benalcazar, T. L. Hughes, and G. Bahl, Nature 555, 346 (2018).
[43] S. Imhof, C. Berger, F. Bayer, J. Brehm, L. W. Molenkamp, T. Kiesling, F. Schindler, C. H. Lee, M. Greiter, T. Neupert, and R. Thomale, Nature Physics 14, 925 (2018).
[44] C. W. Peterson, T. Li, W. A. Benalcazar, T. L. Hughes, and G. Bahl, Science 368, 1114 (2020).
[45] T. Hofmann, T. Helbig, C. H. Lee, M. Greiter, and R. Thomale, Phys. Rev. Lett. 122, 247702 (2019).
[46] G. Chen, A. L. Sharpe, E. J. Fox, Y. H. Zhang, S. Wang, L. Jiang, B. Lyu, H. Li, K. Watanabe, T. Taniguchi,
SUPPLEMENTARY MATERIALS FOR “ANOMALOUS BULK-BOUNDARY CORRESPONDENCE IN DIMERIZED TOPOLOGICAL INSULATORS”

In main text, we investigate two kinds of topological insulator states in the extended 2D SSH model, hosting anomalous bulk-boundary correspondence. At half-filling, we find a $\mathcal{C} = 2$ Chern insulating (CI) state. With open boundary condition, the in-gap states are divided into two parts—one diffuses into the quasi-edge and the other gathers around the corner, yielding the isolated corner states but without fractional corner charge and the metallic near-edge states. Those exotic boundary states significantly differ from the conventional CIs, which host the well-edge localized boundary states. We identify the present CI by the Wannier bands, and find the shift of the Wannier bands, which further supports the anomaly. Moreover, we find another topological state with zero Chern number at quarter-filling. In this topological state, the boundary states bypass the corner and localize robustly along the edges, yielding the absence of the corner states. In the supplement, we show more details of the topological invariants, characterization of our present topological states, and the robustness of the topological states, etc.

**FIG. S1.** (color online). Evolution of the boundary states with various $v$. (a) Schematic scheme to calculate the real-space Chern number by Kitaev formula by dividing the bulk into three distinct neighboring regions marked with “A”, “B” and “C”. (b)-(f) the spatial distribution of the in-gap states in the $\mathcal{C} = 2$ CI states. $v = 1.0$ for (b) and (c), $v = 1.5$ for (d) and (e), and $v = 2.0$ for (f). Here, $w' = 0.75$ and $\phi = -0.25\pi$.

**Topological invariants**

Topological invariant is an important index to characterize the topological properties of system. Here, we show details of topological invariants used in the main text, including the Chern number, the real-space Chern number,
Wannier centers and 2D Zak phase.

The Chern number \( C_n \) can be calculated by integrating the Berry curvature \( F_n(k) \) over the first Brillouin zone \([11, 34]\),

\[
C_n = \frac{1}{2\pi} \int_{BZ} d^2k F_n(k). \tag{S1}
\]

Here, \( F_n(k) = \nabla \times A_n(k) \) with the berry connection \( A_n(k) = -i\langle u_{nk}|\nabla k|u_{nk}\rangle \) and \( |u_{nk}\rangle \) is Bloch wave functions of the \( n \)th band. Chern number can be expressed in inversion systems at high symmetric points \([38, 39]\) as,

\[
(-1)^C = \prod_i^n \zeta_i(\Gamma)\zeta_i(X)\zeta_i(Y)\zeta_i(M), \tag{S2}
\]

where \( \zeta \) indicates the parity, the eigenvalue of inversion operator \( P \), \( n \) is the number of occupied bands.

The topological characterization of CIs without translational symmetry can be further identified by the real-space Chern number. In the main text, we adopt Kitaev formula to calculate real-space Chern number, i.e.,

\[
C_R = 12\pi i \sum_{j \in A} \sum_{k \in B} \sum_{l \in C} (P_{jk}P_{kl}P_{lj} - P_{jl}P_{lk}P_{kj}). \tag{S3}
\]

A circle region is chosen in bulk and cut into three distinct neighboring regions arranged in a counterclockwise order, marked with “A”, “B” and “C” [Fig. S1 (a)]. \( j, k \) and \( l \) mark the sites in \( A, B \), and \( C \) regions, respectively \([36]\). \( \hat{P} \) is the projection operator defined up to Fermi energy \( E_F \) and \( \hat{P} = \sum_{E_n < E_F} |\phi_n\rangle \langle \phi_n| \) with the matrix elements \( P_{ij} = \sum_{E_n < E_F} \phi_n(r_j)\phi_n^*(r_i) \).

We compute the Wannier centers of the present CI states in the main text. Wannier centers can be implemented with the aid of the Wilson loop \([20, 21]\). In the thermodynamic limit, Wannier bands along \( k_y \) are obtained based on the Wilson loop operator \([20, 21]\),

\[
W_{(k_x + 2\pi k_y)\rightarrow (k_x, k_y)} = \lim_{n \rightarrow \infty} [F_{n-1} \ldots F_1 F_0]. \tag{S4}
\]

Here, \( [F_t]_{mn} = \langle u_m(k_{i+1}, k_y)|u_n(k_i, k_y)\rangle \) is the \( n \)-th eigen wave-function, \( k_i = \frac{2\pi n_i}{N} \) and \( m, n = 1, 2 \ldots N_{occ} \).

By diagonalizing these Wilson loop operators, we obtain the Wannier spectra on the torus geometry. Since the Wilson loop operator is unitary \([20, 21, 26]\), the eigenvalue equation can be written as,

\[
W_{x,k} |\nu^j_{x,k}\rangle = \exp(2\pi i\nu^j_{x,k}) |\nu^j_{x,k}\rangle, \tag{S5}
\]

where \( \nu^j_{x,k} \) corresponds to the Wannier center of the \( j \)th Wannier function and determines the Wannier bands.

The zero-Chern number topological state in dimerized lattice with inversion symmetry is characterized by the 2D Zak phase or wave polarization, which is expressed based on the parity as \([33, 39]\),

\[
p_i = \sum_n p_i^n, \quad p_i^n = 1/2(q_i^n \mod 2), \quad (-1)^n = \frac{\zeta(X_i)}{\zeta(\Gamma)}, \tag{S6}
\]

where \( i \) denotes \( x- \) or \( y- \) direction.

\[ C = 2 \text{ CI states} \]

For a weak dimerized potential \( v = 1.0 \) and \( v = 1.5 \), some of boundary states are robustly localized along the edges [Fig. S1 (b) and (d)], in analogy to the conventional CIs. However, other boundary states bypass the corners and slightly extend into the near-edges [Fig. S1 (c) and (e)], which is in contrast to the conventional CIs (Fig. S2).

When the boundary states robustly localized along the edges [Fig. S1 (b) and (d)], a weak but visible portion gathers at corners even at weak \( v \). The corner states enhances with \( v \) [Fig. S1 (f) at \( v=2.0 \)]. When \( v > 2.2 \), the isolated corner states and the near-edge states are evident.

For strong dimerization, the boundary states gather at corners and diffuse into quasi-edge, even in the strong dimerization limit. We show the spatial distribution of the 800th state (edge state) in a 1600-site square lattice with \( v = 20.0 \) and \( v = 50.0 \) in Fig. S3 (a) and (b). Evidently, the above mentioned features of the boundary states remain robust. The corner charge of the present CI state is further calculated, and no fractional corner charge is observed.
FIG. S2. (color online). Edge states of conventional CIs. We present the robust edge states of (a) Checkerboard model, (b) Haldane model with Chern number $C = 1$ and (c) Haldane model with Chern number $C = 2$.

FIG. S3. (color online). The distributions of the anomalous boundary at half-filling in the strong dimerization limit. (a) $v = 20.0$ and (b) $v = 50.0$. There is no excessive charge around the corners in (c) and (d) when $v = 20.0$ and $v = 50.0$. Here, $w' = 0.75$ and $\phi = -0.25\pi$.

FIG. S4. (color online). Eigen-energies and distribution of boundary state in real-space. Here, we choose a $20 \times 20$ square lattice with a defect. (a) Eigen-energies $E$ versus the state index with $v = 5.0$ and 10.0. And we plot the distributions of boundary states with $v = 5.0$ in (b) and $v = 10.0$ in (c). The hopping and flux parameters are chosen as $w' = 0.75$ and $\phi = -0.25\pi$.

Hence, this provides a proof to identify the topological state as a CI state, instead of the higher-order topological insulator (HOTI) state.

In order to check the robustness of the present CI state, we introduce some defects and consider the eigenstate in
real-space. Here, we show the energy levels and the distribution of topological state in Fig. S4. The isolated corner states, as well the near-edge states, remain robust. Around the defects, the additional corners states and near-edge states emerge, manifesting the robustness of the topological boundary states against the defects [Fig. S4 (b) and (c)]. The boundary states are also robust against the large enough lattice size, the coexistence of isolate corner states and near-edge states are observed in $40 \times 40 \times 4$, $50 \times 50 \times 4$ and $60 \times 60 \times 4$ lattices as shown in Fig. S5.

![Figure S5](image)

**FIG. S5.** (color online). Robustness of the CI state against size effect. We consider various sizes of square lattice with (a) $40 \times 40 \times 4$, (b) $50 \times 50 \times 4$ and (c) $60 \times 60 \times 4$ sites. Here, The hopping and flux parameters are chosen as $v = 10.0$, $w' = 0.75$ and $\phi = -0.25\pi$.

![Figure S6](image)

**FIG. S6.** (color online). Wannier bands of (a) normal insulators with $v = 0.5$, (b) CI-like metallic phase with $v = 1.0$ and (c) the second ATI phase with $v = 3.0$. In (d), the Wannier bands of 2D SSH model with $v = 3.0$. The hopping and flux parameters of our model are chosen as $w' = 0.75$ and $\phi = -0.25\pi$.

### Zero-Chern number topological states

As the topological invariant, the Wannier bands in the HOTIs are gapped out [20, 21, 26]. On the other hand, CIs host a gapless Wannier bands, and the Chern number can be obtained from the Wannier centers [21]. We have shown the Wannier centers of conventional CIs and the present CI state in the main text. Here, we show the Wannier bands
of the proposed topological state at 1/4-filling, together with that in the normal insulator state with \( v = 0.5 \), the Chern-like metallic state \( v = 1.0 \). The Wannier centers \( \nu(0) = \nu(\pi) = \nu(2\pi) = 0 \) in the normal insulator and others are near zero [Fig. S6 (a)]. In comparison, the Wannier centers in the metallic CI-like phase are similar to the CIs, where the gapless Wannier bands with \( \nu_x(0) = 0, \nu_x(\pi) = 0 \) and \( \nu_x(2\pi) = -0.5 \) is observed [Fig. S6 (b)]. However, due to the indirect gap between the first and the second bands shown in main text, it is more likely a metallic state. For the zero-Chern number topological state (\( v = 3.0 \)), the Wannier bands are gapped out, in agreement with the missing corner states shown in main text. The Wannier centers [Fig. S6 (c)] is similar to a novel topological state reported in the previous 2D SSH model [33] [Fig. S6 (d)] with \( \nu_x(0) = 0, \nu_x(\pi) = \pm 0.5 \) and \( \nu_x(2\pi) = -0.5 \). Hence, we can use these special Wannier bands and Wannier centers to identify various topological phases.

![FIG. S7. Bulk energy bands along the high symmetric direction at fixed \( w' = 0.75 \). (a). \( v = 5.0, \phi = 0 \), (b). \( v = 1.0, \phi = 0.25\pi \). The parity at the high symmetric points (\( \Gamma, X \) and \( M \)) is denoted by \( \pm \).](image)

In additional, this zero-Chern number topological state can be identified by the 2D Zak phase [33], which can be implemented based on the parity. We show the parity at each high symmetric points, marked with \( \pm \) in Fig. S7. When \( v = 5.0, w' = 0.75 \) and \( \phi = 0 \), the parity of each band is the same as the topological state in 2D SSH model [33]. The parity of the lowest band remains unchanged at \( \phi = 0.25\pi \). Therefore, no phase transition occurs, which can be further verified with the aid of the evolution of the energy gaps with \( \phi \) [Fig. S8(a)]. Based on Eq. S2, we obtain the Chern number of the lowest band is zero. However, based on the Eq. S6, the wave polarization is \( (p_x, p_y) = (1/2, 1/2) \), which suggest that the 2D Zak phase is \( (\pi, \pi) \). Without lattice dimerization, i.e., \( v = 1.0 \), the parity in \( M \)-point changes the sign, and the Chern number at 1/4-filling is \( C = 1 \), however, there is no energy gap between the two lowest bands.

We check the eigen-energies of the first and the second energy bands versus the staggered flux \( \phi \) on the torus. No band crossing by tuning \( \phi \) is observed [Fig. S8(a)], which indicates no phase transition. Therefore, the topological state at \( \phi = 0 \) observed previously in the 2D SSH model and the topological state reported here belong to the same topological class, though the time reversal symmetry is preserved, and is broken in the former, and in the latter, respectively. We further show the robustness of this topological state with \( v = 5.0 \) and \( v = 10.0 \) in Fig. S8 (b) and (c). This topological state is very robust for the boundary states bypassing the defect.

![FIG. S8. (color online). (a). Eigen-energies \( E \) versus the staggered flux \( \phi \) on the torus geometry. (b) \( v = 5.0 \) and (c) \( v = 10.0 \) are the distributions of the zero Berry curvature topological state in a square lattice with defect. The hopping and flux parameters are chosen as \( w' = 0.75 \) and \( \phi = -0.25\pi \).](image)