Topological Wannier cycles in $C_3$ and $C_2$ symmetric insulators

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Abstract

Recently, with the discovery of various higher-order topological insulators, such spectral topological characteristics are extended from edge states to corner states. However, the chiral symmetry protecting the corner states is often broken in most materials, leading to vulnerable corner states even when the topological invariants remain well-defined. Here, we propose a single-plaquette artificial gauge flux insertion as a robust spectral probe of higher-order topological insulators which is effective even when the chiral symmetry is broken. The artificial gauge flux leads to the topological Wannier cycles that emerge essentially due to the cyclic transformation of the Wannier orbitals composing the energy bands. Topological Wannier cycles are cyclic spectral flows, as demonstrated here in $C_3$ and $C_2$ symmetric insulators, when the local gauge flux is acting on the Wannier orbitals. Therefore, topological Wannier cycles probe the location of Wannier orbitals and discern various Wannier-type higher-order topological phases.

Introduction

The discovery of higher-order topological insulators (HOTIs) generalizes the celebrated bulk-edge correspondence [1, 2] to various multidimensional bulk-boundary correspondences [3-11], such as the bulk-edge-corner correspondence. For instance, in two-dimensional (2D) HOTIs, the emergence of zero-dimensional (0D) corner states in the bulk band gap is often used as a spectral signature of the multidimensional topological physics and the higher-order topology. Such a phenomenon, though convenient for experimental measurements [12-32],
however, has deficiencies. Due to chiral symmetry breaking in most materials, the frequencies of the corner states are not pinned to the middle of the bulk band gap. Under certain situations, these corner states can even be tuned out of the bulk band gap and merge into the bulk bands [33]. In these situations, the spectral probe of the higher-order topology becomes impossible, making the detection of the higher-order topology relying on the detection of the fractional corner charges [11, 34, 56] which are much more difficult to measure in experiments.

Here, we propose a way to create a highly localized, single-plaquette artificial gauge flux $\Phi$ that embraces the full gauge phase range of $0$ to $2\pi$ and argue that such an artificial gauge flux can be a powerful tool to probe the higher-order band topology, or generally speaking, the filling anomaly and fractional charges [11]. Most importantly, the local gauge flux induces topological Wannier cycles in HOTIs that are Wannier representable (i.e., having well-defined Wannier centers [35-38]). This emergent effect, which is the center of this paper, is due to the cyclic evolution of the Wannier orbitals at the same Wyckoff position but of different symmetries. These Wannier orbitals compose the energy bands above and below the band gaps. Topological Wannier cycles are manifested as the cyclic spectral flows that traverse one or multiple band gaps when the single-plaquette gauge flux encloses the Wannier centers and acts on the Wannier orbitals. These spectral flows evolve from bulk states at $\Phi = 0$ and $\Phi = 2\pi$, and gradually become localized states bound to the local gauge flux in the bulk band gaps. Topological Wannier cycles are protected by the crystalline and time-reversal symmetries and are dictated by the real-space topological invariants (RSTIs) [10, 39, 40]. The RSTIs connect the filling anomaly of the bulk bands with the topological Wannier cycles. Since the filling anomaly dictates the fractional corner charges [11], our study thus establishes topological Wannier cycles as a topologically protected, gapless spectral signature of 2D HOTIs.

**HOTIs with various symmetry**

The topological Wannier cycles in HOTIs are previously elaborated in the 2D Su-Schrieffer-Heeger (SSH) model with four-fold ($C_4$) rotation symmetry using designed sonic crystals [55]. Here, without loss of generality, we revisit another two prototype models that are defined for spinless particles on lattices with three-fold ($C_3$) and two-fold ($C_2$) rotation symmetry. These tight-binding (TB) models are introduced in Fig. 1, where, a breathing kagome model realizes the HOTI with $C_3$ rotation symmetry [see Fig. 1(a)]. As a special case, we also consider the 2D SSH model as the simplest model with $C_2$ rotation symmetry. Here, the 2D SSH model is constructed by weakly coupling the one-dimensional (1D) SSH chain
along the vertical direction [see Fig. 1(c)]. Although such the 2D SSH model should not be classified as a HOTI, it has well-defined Wannier centers and filling anomaly which can thus serve as a particularly simple case to illustrate the topological Wannier cycles.

![Image](image_url)

**Fig. 1 |** (Color online) (a) and (b) Schematic illustrations of the 2D breathing kagome lattice with $C_3$ symmetry and the 2D SSH model with $C_2$ symmetry. (c) and (d) Band structures and symmetry properties of the bands for the TB models in (a) and (b), separately. For each figure, the left panel indicates the trivial phase while the right panel indicates the topological phase. Insets illustrate the location of the Wannier centers in a unit-cell. Symbols represent the little group representations at the high-symmetry points of the Brillouin zone. Symbols in colored circles are used to highlight the different symmetry properties between the trivial and topological phases. The TB parameters are listed above each panel.

We first give the energy bands and their properties for these TB models in both the topological and the trivial phases. The Wannier orbitals of these energy bands are illustrated in Fig. 2. As shown in Fig. 1(b), the breathing kagome model has three bands separated by one energy gap. These energy bands are composed of Wannier orbitals with different $C_3$-rotation eigenvalues, $g_n^{(3)} = e^{i n \pi / 3} (n = 0, 1, 2)$ [see Fig. 2(a)]. In the trivial phase, the Wannier centers (i.e., the center of the Wannier orbitals) of all bands locate at the unit-cell center. In contrast, in the topological phase, the Wannier centers locate at the corners of the unit-cell. The trivial phase is realized when the intra-unit-cell coupling $t_1$ is stronger than the inter-unit-cell coupling $t_2$, while the topological phase is realized when the inter-unit-cell coupling $t_2$ is stronger than the intra-unit-cell coupling $t_1$. 
Similarly, for the 2D SSH model, if the inter-unit-cell $t_2$ is stronger than the intra-unit-cell coupling $t_1$, the system is in the topological phase and the Wannier centers are at the edge of the unit-cell. Reversing the inter-unit-cell and the intra-unit-cell couplings leads to the trivial phase where the Wannier centers are at the unit-cell center. There are two bands separated by one energy gap, which originate from two Wannier orbitals with different $C_2$-rotation eigenvalues, $g_n^{(2)} = e^{\frac{in\pi}{2}}$ ($n = 0, 1$) [see Fig. 2(b)].

![Fig. 2 | (Color online) Wannier orbitals in the breathing kagome lattice model (a) and the SSH model (b).](image)

The phase differences between adjacent petals indicate the rotation symmetries $g_n^{(3)} = e^{\frac{in\pi}{2}}$ with $n = 0, 1, 2$ in (a) and $g_n^{(2)} = e^{\frac{in\pi}{2}}$ with $n = 0, 1$ in (b).

**Single-plaquette artificial gauge flux**

We now create the single-plaquette artificial gauge flux from three consecutive procedures. These procedures are illustrated in Fig. 3(a). The first procedure is dimension extension. For instance, the 2D breathing kagome model is stacked along the $z$-direction periodically to extend the system from a 2D model to a three-dimensional (3D) model. Note that here the coupling in the $z$-direction is not essential. We, in fact, consider the limit that the coupling along the $z$-direction vanishes. We then create a step screw dislocation at the center of these dimension-extended systems. We specifically consider systems that are finite in the original dimensions but periodic in the $z$-direction for the breathing kagome model. Here, the step screw dislocation consists of three flat sectors (“steps”). But the couplings between the adjacent sectors are tilted in such a way that these flat steps form a screw dislocation with a clear chirality. Particularly, in our calculations, the system has $3N(3N - 1)/2$ unit-cells (with $N = 10$) in the $x$-$y$ plane where the dislocation core is at the center of this plane [see Fig. 3(b)]. Therefore, each sector has $N(3N - 1)/2$ unit-cells. Such a designed system has an emergent screw symmetry $S_{3z} = C_3 \ast L_z(\frac{1}{3})$ with $L_z(\frac{1}{3})$: $z \rightarrow z + \frac{1}{3}$ (we set the lattice constants along all directions as unit for the TB models in this work) which play a pivotal role in the emergent physics.
For the dimension-extended 2D SSH model, we can create a step glide dislocation that is finite in the $x$-direction and periodic in the $y$- and $z$-directions [see Fig. 3(c)]. The system then has an emergent glide symmetry $G_{2z} = C_2 \ast L_z (\frac{1}{2})$ with $C_2 := x \rightarrow -x$.

After the dimension extension and the creation of the dislocations, we now employ the dimensional reduction procedure. Dimensional reduction [53] is a tool to map higher dimensional physics into lower dimensional physics which is widely used in the study of topological physics. Here, this procedure is achieved by the Fourier transformation along the $z$-direction. After the Fourier transformation, the dimension along the $z$-direction becomes a system with parameter $k_z$ and thus leads to the reduction of dimension by one.

The effective models after the three consecutive procedures are given in Figs. 3(d) and (e). Due to the Fourier transformation along the $z$-direction, each tilted coupling between the adjacent sectors will pick up a gauge phase factor $e^{i\theta}$ along the arrows indicated in Figs. 3(d) and (e). This gauge phase is $\theta = \frac{k_z}{3}$ or $\frac{k_z}{2}$, separately for the 2D breathing kagome model and the 2D SSH model. With the gauge phase configurations illustrated in Figs. 3(d) and (e), the highly localized artificial gauge flux confined in a single-plaquette, $\Phi = k_z \in [0, 2\pi]$, emerge at the center of the system for the breathing kagome model. Note that in this work, we
abbreviate the gauge flux as a phase which is adequate to capture the essential physics in the studied systems. For the 2D SSH model, the localized artificial gauge flux can be regarded as to be confined in the center of each SSH chain [see the top panel in Fig. 3(e)].

Topological Wannier cycles induced by the local gauge flux

We now show that the single-plaquette artificial gauge flux can lead to the topological Wannier cycles. The key here is to understand the cyclic transformation of the Wannier orbitals under the local gauge flux insertion. For instance, for the breathing kagome model, the three bands are made of three Wannier orbitals with the $C_3$-rotation eigenvalues, $g_n^{(3)} = e^{i n \pi / 3}$ ($n = 0, 1, 2$). The artificial gauge flux $\Phi$ acts only on the Wannier orbitals in the central plaquette, then these Wannier orbitals now have the $C_3$-rotation eigenvalues, $e^{i n (\pi n / 3) + \Phi / 3}$. This change can also be understood by replace the $C_3$ rotation to the $S_{3z}$ rotation in the structure with a step screw dislocation. Since $S_{3z} = C_3 \ast L_z (\frac{1}{3})$, the $C_3$-eigenstates at $k_z$ pick up an additional phase, $e^{i k_z / 3} = e^{i \Phi / 3}$, due to the translation along the $z$-direction $L_z (\frac{1}{3})$. When a $\Phi = 2\pi$ gauge flux is inserted in the central plaquette, the rotation eigenvalues transform as, $g_n^{(3)} \rightarrow g_{n+1}^{(3)}$. Because $n = 0, 1, 2$ is a modulo 3 quantity, such transformation forms a closed cycle, $g_0^{(3)} \rightarrow g_1^{(3)} \rightarrow g_2^{(3)} \rightarrow g_0^{(3)}$. Since each Wannier orbital comprises and represents a bulk band, the cyclic transformation among the Wannier orbitals leads to a cyclic spectral flow among the bulk bands [see Fig. 4(c)], which is exactly the topological Wannier cycles. In contrast if the system is trivial, e.g., $t_1 = -1$ and $t_2 = 0.5$, then the Wannier orbitals live on the plaquettes that do not carry any gauge flux, and the inserted gauge flux thus has no effect on the spectrum.

The Aharonov-Bohm principle [54] states that essentially the gauge flux induces a change in the phase of the wavefunctions. Normally, inserting a gauge flux $\Phi = 2\pi$ has no physical effect, since the phase $2\pi$ is equivalent to the phase $0$. However, in topological systems, inserting a gauge flux $\Phi = 2\pi$ can lead to nontrivial effects. The topological Wannier cycle is one of the nontrivial effects that can emerge in topological crystalline systems.

We now analyze the filling anomaly of the breathing kagome model. Consider a triangular, finite 2D system with $3N(3N - 1)/2$ unit-cells without the artificial gauge flux. Such a finite system has the $C_3$ rotation symmetry, while the lattice translation symmetry is broken. In the trivial case, because the Wannier orbitals are at the unit-cell center, there are $3N(3N - 1)/2$ bulk states in each bulk band.
In the topological case, the filling anomaly emerges, the situation is quite different. We find that there are \(9(N - 1)\) edge states in each band gap. In addition, there are two sets of threefold-degenerate corner states whose total energy is pinned to zero due to the higher-order topology and chiral symmetry. Most importantly, there are \(\frac{9N(N-1)}{2} + 1\) bulk states in the first bulk band. This number of bulk states is a consequence of the band topology and has several highly nontrivial features. First, it predicts a fractional corner charge. Since the finite system is \(C_3\)-symmetric, each quarter sector then has \(\frac{3N(N-1)}{2} + \frac{1}{3}\) states. Therefore, filling the first bulk band leads to a fractional corner charge of \(e/3\) or \(-2e/3\), where \(e\) is the electron charge.

Second, the number of bulk states also dictates the topological Wannier cycles. Because when a \(\Phi = 2\pi\) gauge flux is inserted into the central plaquette, the eigenstates transform cyclically, as illustrated in Fig. 4(a). This cyclic transformation must be completed within a group of three eigenstates. However, the number of bulk states in the first bulk band, \(\frac{9N(N-1)}{2} + 1\), is not an integer multiple of three. Simultaneously, there are two bulk states above the gap which cannot find their partner as well. Therefore, the cyclic transformation of eigenstates cannot be fulfilled within the first bulk band. Consequently, there must be a cyclic transformation of eigenstates among different bulk bands across the band gaps, which is just the emergent topological Wannier cycles shown in Fig. 4(c) [also depicted in the right panel of Fig. 4(a)]. The energy spectrum in Fig. 4(c) is obtained from the calculation based on the TB model in Fig. 3(d). It is seen that the edge and corner states appear in the band gap, yet they do not evolve with the inserted gauge flux and have nothing to do with the spectral flows and the topological Wannier cycles. We emphasize that since the numbers of the edge and corner states are both integer multiples of three, whether these states are filled or not does not change the above reasoning.
Fig. 4 | (Color online) Topological Wannier cycles in the breathing kagome and SSH models. (a) and (b): Schematic illustration of the transformation of the eigenstates due to the single-plaquette gauge flux insertion $\Phi = k_z$. The eigenstates are labeled by either the $C_3$-rotation eigenvalues $g_n^{(3)} = e^{in(2\pi/3)}$ with $n = 0, 1, 2$ for (a) the breathing kagome model, or the $C_2$-rotation eigenvalues $g_n^{(2)} = e^{in(\pi/2)}$ with $n = 0, 1$ for (b) the SSH model. The rotation eigenvalues of the eigenstates evolve cyclically when $\Phi$ goes from 0 to $2\pi$. The right panels give the schematic illustrations of the emergent cyclic spectral flows across the band gaps induced by the local gauge flux insertion. (c) and (d): The energy spectra of the TB models as functions of the artificial gauge flux $\Phi = k_z$ for the finite systems in Fig. 3(d) and in Fig. 3(e). The TB parameters are $t_1 = -0.5$, $t_2 = -1$ and $N = 10$ in both (c) and (d). Here, the energy spectra in (d) is calculated for the SSH model finite in the $x$-direction and periodic in the $y$-direction with a vertical coupling $t_3 = -0.2$ and $k_y = 0.5\pi$. The grey and green regions denote the bulk and edge states, respectively. The orange curves with red arrows represent the spectral flows between the bulk bands. The blue lines in (c) and (d) denote the corner states of the breathing kagome model and edge states of the SSH chain. Both the edge and corner states have nothing to do with the spectral flows across the band gaps, i.e., the topological Wannier cycles.

Closer examination of the spectral flows indicates that at $\Phi = 0$ the system returns to the breathing kagome model. The spectral flows start from the bulk states in the $\Phi = 0$ limit and evolve gradually into the localized states bound to the artificial gauge flux at the central plaquette. At $\Phi = \pi$, two time-reversal symmetric topological boundary states become degenerate due to the fact that the $C_3$-rotation eigenvalues of the topological boundary states are mutually conjugated. At $\Phi = 2\pi$, the spectral flow ends at a bulk band that is different from the original bulk band it starts from. The cyclical spectral flows perfectly satisfy the periodicity
as $\Phi = k_z$ goes from 0 to $2\pi$, yet with the connections determined by the bulk invariants (see analysis below), they manifest the nontrivial topological spectral evolutions across the band gaps.

The above analysis shows that the number of eigenstates in each bulk band is a crucial indicator of the higher-order band topology. More precisely, the number of eigenstates modulo three for all the bulk bands below the concerned band gap is the true indicator. We now connect this indicator with the bulk topological invariants which are called as the real-space topological invariants (RSTIs). The theory of RSTIs is proposed and developed in Refs. [10, 39, 40]. The RSTIs are good quantum numbers in real space that connect to the symmetry indicators of the Bloch bands [35-38] and the topological invariants (such as the Chern and $Z_2$ numbers) related to the symmetry indicators [35]. For a finite $C_3$-symmetric 2D system, the eigenstates have three irreducible representations (IRs), i.e., $A$, $^2E$, and $^1E$, corresponding to the three $C_3$-rotation eigenvalues $g_n^{(3)} = e^{in\frac{\pi}{3}}$ with $n = 0$, 1 and 2 mod 3, separately. The RSTIs are defined as the following three integer invariants

$$ (\delta_1, \delta_2) = (m(g_2) - m(g_0), m(g_1) - m(g_0)) \text{.} $$

Here, $\delta_2$ is equal to $\delta_1$ in the presence of time-reversal symmetry. $m(g_n)$ denotes the multiplicity of the eigenstates with $C_3$-rotation eigenvalue $g_n$ for the finite system. Interestingly, although the above definition is based on finite systems, the RSTIs can be deduced from the symmetry indicators of the Bloch bands below the concerned band gap at the high-symmetry points (HSPs) in the Brillouin zone [39]. In our $C_3$-symmetric system, the RSTIs are calculated as follows [39],

$$
\begin{align*}
\delta_1 &= \frac{2}{3}m(^2E_\Gamma) + \frac{1}{3}m(^1E_\Gamma) - m(A_K) - m(^2E_K), \\
\delta_2 &= \frac{1}{3}m(^2E_\Gamma) + \frac{2}{3}m(^1E_\Gamma) - m(^2E_K) \text{.}
\end{align*}
$$

Here, the symbols in the bracket represent the IRs at the HSPs in the Brillouin zone (the HSPs are the $\Gamma$, $M$, and $K$ points which are represented by the subscripts). The $m$’s denote the multiplicity of the IRs below the band gap. For instance, $m(A_K)$ denotes the multiplicity of the IR $A$ at the $K$ point. Based on the IRs labeled at the HSPs in Fig. 1c, the RSTIs of the band gap is calculated as $(-1, -1)$ and $(0, 0)$ for the topological and trivial cases, respectively.

Using the above RSTIs, we find that, for the process with $\Phi = k_z$ varying from 0 to $2\pi$, the imbalance of the bulk eigenstates in the topological case is given by $\Delta(g_0) = m(g_2) - m(g_0) = \delta_1 = -1$, $\Delta(g_1) = m(g_0) - m(g_1) = -\delta_2 = 1$ and $\Delta(g_2) = m(g_1) - m(g_2) = \delta_2 - \delta_1 = 0$. This implies that there is one excess bulk state with the IR $A$ below the band gap
and two excess bulk states with the IRs \(2E\) and \(1E\) above the band gap. The nonzero \(\Delta(g_0)\) and \(\Delta(g_1)\) account for the cyclic transformation of excess bulk states that cannot find their partners within the bulk bands they belonged to. The resultant spectral flow across the band gap is presented in Fig 4(c).

We now turn to the analysis of the SSH model. We consider a semifinite system with \(2N\) unit-cells along the \(x\)-direction (periodic in \(y\)- and \(z\)-directions), as depicted in Fig. 3(e). This finite system has \(C_2\) rotation symmetry and can thus be divided into two symmetric sectors. After the Fourier transformation for both \(y\)- and \(z\)-directions, there are \(2N - 1\) bulk states in each bulk band in the finite system in the topological phase (we consider the system at specific \(k_y\)). For comparison, in the trivial phase, there are \(2N\) bulk states in each bulk band. In the topological phase, there are two edge states in the bulk band gap.

Because of the strange number of bulk states below the band gap, each sector has a fractional charge of \(e/2\) if the bulk states below the band gap are all filled, because the filling of the first bulk band yields \(N - \frac{1}{2}\) bulk states in each sector. Notice that since there are two edge states in the bulk band gap, whether they are filled or empty, they do not affect the fractional charge. This fractional charge is known for decades but observed only recently [56].

The strange number of the bulk states in each band is also reflected by the topological Wannier cycles. Inserting a gauge flux at the center of the 2D SSH model leads to the cyclic transformation between the states of different IRs, \(A\) and \(B\) (or equivalently, \(g_0^{(2)}\) and \(g_1^{(2)}\), i.e., \(g_0^{(2)} \rightarrow g_1^{(2)} \rightarrow g_0^{(2)}\) [see Fig. 4(b)]. Since each band has \(2N - 1\) bulk states, there is one bulk state having no partner of transformation within the bulk band it belongs to. Therefore, there must be a cyclic transformation formed by two states belong to different bulk bands. Such cyclic transformation leads to the topological Wannier cycle which is manifested as the spectral flows across the band gap. This topological Wannier cycle is realized by the glide step dislocation in Fig. 3(c). The energy spectrum that confirms the emergent topological Wannier cycle explicitly is given in Fig. 4(d) which is obtained from the calculation based on the TB model in Fig. 3(e).

The RSTI for our \(C_2\)-symmetric 2D SSH model is defined as a single number [39],

\[
\delta = m(g_1) - m(g_0).
\]

Similarly, it can be calculated as follows in terms of the IRs at HSPs in momentum space [39],

\[
\delta = -\frac{1}{2} m(A_T) - \frac{1}{2} m(B_X).
\]
We find $\delta = -1$ for the topological band gap. It implies that the states with $C_2$-rotation eigenvalues $g_0$ and $g_1$ redundant in two different bands transform cyclically in the band gap. For the trivial band gap, we find $\delta = 0$ and thus no spectral flow emerges.

The above analysis for both the the breathing kagome model and the SSH model establishes a firm connection between the filling anomaly (or equivalently the fractional charge) and the topological Wannier cycles. We emphasize that unlike the corner states protected by the chiral symmetry which are commonly used as a signature of higher-order topology, the filling anomaly does not rely on the chiral symmetry. In fact, breaking chiral symmetry does not affect the above analysis and reasoning. Thus, the topological Wannier cycles are robust against chiral symmetry breaking. As shown in a recent experiment [55], topological Wannier cycles can emerge in phononic systems where the chiral symmetry is broken. Intriguingly, in such phononic systems, chiral symmetry breaking destroys the edge and corner states, yet the topological Wannier cycles remain as a salient spectral feature with robust, gapless topological boundary states [55].

**Conclusion and outlook**

We propose a mechanism for realizing single-plaquette artificial gauge flux via the procedures involving dimension extension, introducing a step screw dislocation and dimensional reduction. Through such highly localized artificial gauge flux, we show that a cyclic transformation of the eigenstates in finite systems can be induced. When the lattice system is in the higher-order topological phases that are Wannier representable, such artificial gauge flux insertion leads to emergent topological Wannier cycles that are manifested as cyclic spectral flows across the band gaps. These gapless spectral flows are revealed to be gapless topological boundary states propagating along the $z$-direction and bound to the single-plaquette gauge flux. We establish a firm connection between filling anomaly and topological Wannier cycles and thus reveal that topological Wannier cycles are novel gapless spectral features robust against chiral symmetry breaking. We remark that the topological Wannier cycle can also be realized in Floquet systems where the insertion of single-plaquette artificial gauge flux is accessible without the aid of the structural dislocation. Our work unveils an unprecedented topological phenomenon and a regime for the creation of highly localized artificial gauge flux that has not been reached before. Such single-plaquette artificial gauge flux can be valuable in the realization of exotic topological phases as well as in the manipulation of phononic, photonic and electronic waves.
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