Hofstadter Topology: Non-crystalline Topological Materials in the Moiré Era

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The Hofstadter problem is the lattice analog of the quantum Hall effect and is the paradigmatic example of topology induced by an applied magnetic field. Conventionally, the Hofstadter problem involves adding $\sim 10^4$ T magnetic fields to a trivial band structure. In this work, we show that when a magnetic field is added to an initially topological band structure, a wealth of remarkable possible phases emerges. We prove that threading magnetic flux through a Hamiltonian with nonzero Chern number enforces a gapless point within the Hofstadter Butterfly [1]. This system is host to a wealth of nontrivial Chern number topology protected by the product of two-fold rotation and time-reversal and show that there exists a 3D higher order TI phase where corner modes are pumped by flux. We show that a model of twisted bilayer graphene realizes this phase. Our results rely primarily on the magnetic translation group which exists at rational values of the flux. The advent of Moiré lattices also renders our work relevant experimentally. In Moiré lattices, it is possible for fields of order 1–30 T to reach one flux per plaquette and allow access to our proposed Hofstadter topological phase.

## I. INTRODUCTION

When a two dimensional crystalline lattice in which electrons have a trivial band structure is pierced by a uniform magnetic field, translational symmetry is broken and the energy spectrum develops a complex, fractal structure known as the Hofstadter Butterfly [1]. This system is host to a wealth of nontrivial Chern number topology despite the triviality of the original band structure [2,3]. In this work, we show that the Hofstadter problem acquires new properties when the initial band structure is already topological and demonstrate new phases not possible in crystalline insulators of the same spatial dimension. Specifically, we prove that (1) a nonzero Chern number or mirror Chern number enforces a gapless point in the bulk of the Hofstadter Butterfly and (2) insulators with time-reversal symmetry $\mathcal{T}$ (TRS) and nontrivial $\mathbb{Z}_2$ invariant can be considered as either strong or weak 3D topological insulators (TIs) in flux and host gapless surface states. We then study insulators with fragile topology protected by $C_2,\mathcal{T}$ symmetry (squaring to +1) and (3) show that the Hofstadter Hamiltonian can achieve a 3D Higher Order TI (HOTI) phase characterized by corner mode pumping. We then show that a model of twisted bilayer graphene in magnetic field realizes the HOTI phase [4].

Recently, experimental progress in the manufacture of two dimensional crystals has brought measurements of the Hofstadter Butterfly within reach by synthesizing Moiré lattices with mesoscale effective unit cells such that large fluxes are accessible at laboratory-strength magnetic fields [5,20]. We expect our theoretical predictions to be verifiable in the near future, opening a new field of Hofstadter topology.

First we review the framework for introducing magnetic flux on a lattice using the Peierls substitution [21]. We consider a general tight-binding model with unit vectors $\mathbf{a}_1, \mathbf{a}_2$ whose lattice points we call $\mathbf{R}$, with orbitals at $\delta_\alpha, \alpha = 1, \ldots, N_{\text{orb}}$, and hopping elements given by $t_{\alpha\beta}(\mathbf{r} - \mathbf{r}')$. $\mathbf{r} = \mathbf{R} + \delta_\alpha, \mathbf{r}' = \mathbf{R}' + \delta_\beta$. The number of occupied bands is $N_{\text{occ}}$. We write $c_{\mathbf{R},\alpha}^\dagger$ (resp. $c_{\mathbf{R},\alpha}$) as the the fermion creation (resp. destruction) operator of the $\alpha$ orbital at position $\mathbf{R} + \delta_\alpha$. We find it convenient to work in units where the area of the unit cell, the electron charge $e$, and $h$ are all set to one. By Peierls’ substitution, the hoppings acquire a phase $t_{\alpha\beta}(\mathbf{r} - \mathbf{r}') \rightarrow t_{\alpha\beta}(\mathbf{r} - \mathbf{r}') \exp \left[ i \oint_{\mathbf{R} + \delta_\alpha} \mathbf{A} \cdot d\mathbf{r} \right]$. The path of integration is a straight line between the orbitals when they are well localized (see App. [A]). We work in the Landau gauge $\mathbf{A}(\mathbf{r}) = -\phi \mathbf{b}_1(\mathbf{r} \cdot \mathbf{b}_2)$ where the reciprocal vectors $\mathbf{b}_i$ satisfy $\mathbf{b}_1 \cdot \mathbf{a}_2 = \delta_{ij}$ and $\phi$ is the flux per unit cell. In this gauge, the hoppings retain translation invariance along $\mathbf{a}_1$ but the translation symmetry along $\mathbf{a}_2$ is broken. However, at rational values of the flux where $\phi = \frac{2\pi q}{q}$ with $q, p$ coprime, the hoppings recover an extended translational symmetry: $\mathbf{r} \rightarrow \mathbf{r} + q \mathbf{a}_2$. In this case, we can diagonalize the Hamiltonian in the $1 \times q$ magnetic unit cell:

$$
H^\phi = \sum_{k_1,k_2,\alpha,\beta, r_2' r_2} c_{k_1,k_2,\alpha,\beta, r_2, r_2'}^\dagger \mathcal{H}^\phi(k_1, k_2)|_{r_2, r_2'} c_{k_1,k_2, r_2', \beta}.
$$

(1)

Here $r_2', r_2 = 0, \ldots, q - 1$ are the coordinates of the magnetic unit cell in the $\mathbf{a}_2$ direction, $k_1 \in (-\pi, \pi)$ is the momentum along $\mathbf{b}_1$, $k_2$ is the momentum along $\mathbf{b}_2$ and takes values in $\{0, \frac{2\pi}{q}\}$ due to the enlargement of the magnetic unit cell, and $\mathcal{H}^\phi$ is the single-particle Hamiltonian which we will refer to as the

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Hofstadter Hamiltonian. Although the dimension of $\mathcal{H}^\phi$ is discontinuous in $\phi$, the energy spectrum is continuous (see App. A). Importantly, the Hofstadter Hamiltonian is periodic in flux up to a unitary transformation: $H^{\phi+\Phi} = U H^\phi U^\dagger$, where $\Phi = 2\pi n, n \in \mathbb{N}$ is determined by the condition that all closed hopping loops encircle an integer number of flux quanta. If all orbitals are on the atomic sites and hoppings are along the lattice vectors, then all paths enclose an integer number of unit cells, so $n = 1$. When acting on single-particle states, we can show (see App. A) that

$$U = \sum_{R_0} e^{i \Phi_{R_0}} A \cdot dR_\alpha, \nabla \times \vec{A} = \Phi (2)$$

where $R_0$ is the position of a fixed but arbitrary orbital of the Hamiltonian, and the integral may be taken along any sequence of Peierls paths due to the definition of $\Phi$.

A central feature of the Hofstadter Hamiltonian is the increased periodicity of its Brillouin Zone (BZ) which can be deduced from the magnetic translation group [23]. As shown in Eq. (1), $k_2$ is $2\pi/q$ periodic. Here we show that the energy bands are also $2\pi/q$ periodic along $k_1$. The single-particle magnetic translation operators can be written

$$T_i(\phi) = \sum_{R_0} e^{i \Phi_{R_0}} A \cdot dR_\alpha + i \chi_i(r) \cdot C_{\alpha} \frac{\partial}{\partial \chi_i}, (3)$$

where $\chi_i(r) = \phi a_i \times r$ has been determined by requiring $[H^\phi, T_i(\phi)] = 0$ and the integral is taken along a straight-line path (see App. A). Here we use the convention that the cross product of 2D vectors is a scalar. While the translation operators commute in the absence of flux, otherwise we find $T_1(\phi) T_2(\phi) = e^{i \phi} T_2(\phi) T_1(\phi)$. However, at rational flux $\phi = 2\pi q$, we see $[T_1(\phi), T_2(\phi)] = 0$. A choice of the maximal commuting set is $\{ H^\phi, T_1(\phi), T_2(\phi) \}$ and eigenstates may be written as $|m, k_1, k_2\rangle$ with corresponding eigenvalues $\epsilon_m(\Phi), e^{i \phi}, e^{i \phi_2}$, with $m = 1, \ldots, qN_{orb}$ (see Eq. [1]). Because $[H^\phi, T_2(\phi)] = 0$, the states $T_2(\phi) |m, k_1, k_2\rangle)$ also have energy $\epsilon_m(\Phi)$. The $k_1$ momentum of such states is deduced from the group relation, i.e. $T_1(\phi) T_2(\phi) |m, k_1, k_2\rangle) = e^{i (\phi + \phi_2)} T_2(\phi) |m, k_1, k_2\rangle)$ and hence they may represent the new states at $k_1 + \phi$. Thus we find

$$T_2(\phi) |m, k_1, k_2\rangle \sim |m, k_1 + j\phi, k_2\rangle, \quad j = 0, \ldots, q - 1 (4)$$

are all degenerate in energy. In addition, there is $\frac{2\pi}{q}$ periodicity along $b_2$ due to the reduction of the BZ. We conclude that the BZ has an increased periodicity: $\epsilon_m(\Phi) = \epsilon_m(\Phi + \frac{2\pi}{q})$. This feature is essential in the following proofs. Although the energy is $\frac{2\pi}{q}$ periodic along both $k_1$ and $k_2$, we do not need to reduce the magnetic BZ along $k_1$, i.e. $k_1 \in (0, 2\pi)$ in our Landau gauge (see App. A).

II. CHERN INSULATORS

In this section, we prove that an insulator with nonzero Chern number must have a bulk gap closing in the Hofstadter Butterfly at the Fermi level of the zero-field Hamiltonian. The proof presented here uses only the periodicity of the BZ, but alternative proofs can be deduced from the Wilson loop or for systems with inversion and odd $C^{\phi=0}$ (see App. C).

Consider a Hamiltonian $H^{\phi=0}$ which is gapped with a nonzero Chern number $C^{\phi=0}$ at filling $\nu = N_{occ}/N_{orb}$. We emphasize that the filling is independent of the flux and is fixed throughout. Now we choose a flux $\phi = \frac{2\pi p}{q}$ such that $C^{\phi=0}/q \notin \mathbb{Z}$. Due to the extension of the magnetic unit cell, $H^\phi$ contains $qN_{orb}$ orbitals and $qN_{occ}$ occupied bands at filling $\nu$. First, we introduce an onsite potential term of overall amplitude $M$ to $H^{\phi=0}$ that creates an energy splitting between each of the orbitals. For sufficiently large $M$, the model will be split into $N_{orb}$ trivial bands and it will reach a gapped atomic limit at filling $\nu$ for all $\phi$ (see App. B).

As we increase $M$ to infinity, gap closings occur which eventually cause $H^{\phi=0}/\Phi \neq 0$ to undergo a series of phase transitions into a trivial atomic limit (see App. B) at filling $\nu = q N_{occ}/q N_{orb}$. These closings can be understood with a $k \cdot \mathbf{p}$ model, generically a two band Hamiltonian which in a suitable basis reads $h(k) = d_1(k)\sigma_1 + d_2(k)\sigma_2 + m_3$. The gap closes as $m$ approaches 0 where $d_1(k^*) = 0$. The change in Chern number due to the gap closing is given locally by the $d_i(k^*)$. Now note that if there is gap closing at $k^*$, there must also be an identical gap closing at each of the points $k^* + j\phi b_1$ mod $2\pi, j = 1, \ldots, q - 1$ because of the periodicity in the BZ as established by Eq. (4). Because a multiple of $q$ gap closings separate $H^\phi$ from the trivial atomic limit at large $M$ where the Chern number is zero, it must be that $C^{\phi=0}/q \notin \mathbb{Z}, \text{zero included}$.

Since we chose $q$ such that $C^{\phi=0}/q \notin \mathbb{Z}$, we find by construction that the Chern number has changed during a smooth evolution of the bands. But this is only possible if the gap closes for $\phi \in [0, \frac{2\pi}{q}]$. For every $C^{\phi=0}$, we may choose arbitrarily large $q$ allowing us to conclude that the gap closing must immediately occur when the flux is increased from the fine-tuned point at $\phi = 0$ (see App. C). We stress that if $C^{\phi=0} = 0$, there is no protected gap closing because a vanishing Chern number is possible at all values of the flux. In this case, it is possible to adiabatically add terms that open the gap for all

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1For example, consider a four band Hamiltonian which has $C^{\phi=0} = 1$ at $\nu = \frac{1}{2}$. We can always find a sufficiently large $M$ that trivializes $H^\phi$ for all $\phi$ at filling $\frac{1}{2}$. It is generically not possible to find such an $M$ at other fillings. At $\nu = 1/3$ for instance, this is clearly impossible at $\phi = 0$ because the model has four bands.

2Note that the structure of an onsite potential is identical for the $q$ unit cells within the magnetic unit cell.
φ as long as no other topological or symmetry invariant requires a gap closing.

We now seek to generalize this result for an insulator with a nonzero Mirror Chern number \[24, 25\]. Because mirror symmetry \(M_z\) is not broken in the presence of flux, \(M_z\) remains well-defined at all \(φ\). Then we may block-diagonalize \(H^φ\) at all \(φ\) by its mirror eigenvalues. Each block has a nonzero Chern number at \(φ = 0\), and thus the gap closes immediately at \(φ = 0\) and filling \(ν\) within each individual block. Each block must have a branch of its spectrum connecting its valence and conduction bands. Hence for any Fermi energy in the zero-flux gap, there will be a gapless point at finite flux in the spectrum of the whole model (see App. [3]). In Fig. 1, we consider the Quantum Spin Hall model \(H_{QSH}\) of Ref. [24] with a nonzero Mirror Chern number [24]. We show numerical confirmation that although the Chern number is identically zero (due to TRS), the gap still closes due to the Mirror Chern number.

### III. Time-Reversal Invariant Insulators

We show in this section that when a Hofstadter Hamiltonian with spinful TRS \(T\) is topological (in a quantum spin hall state) at \(φ = 0\), it realizes a nontrivial 3D phase where the flux \(φ\) is identified with \(k_z\). Recall that the Hofstadter Hamiltonian is \(Φ = 2πn\) periodic in flux. When \(n\) is odd, the Hofstadter Hamiltonian is classified as a 3D TI, and may be a weak TI or 3D TI when \(n\) is even. However, it can never be 3D trivial.

The identification of \(φ\) with \(k_z\) is deduced from its transformation under \(T\). Because \(T\) is anti-unitary, it flips the sign of \(φ\) in the Peierls substitution. The Hofstadter Hamiltonian obeys

\[
T^{-1}H^φ(k)T = H^{-φ}(-k) .
\]

Let us first consider the simple case of \(Φ = 2π\), i.e. \(n = 1\). Then \(φ\) is 2π-periodic and behaves as \(k_z\) would in a 3D Hamiltonian. Furthermore, we recall that \(H^φ + T = UH^φU^†\) where \(H^φ\) is the second-quantized Hamiltonian, so from

\[
(U^T)H^φ(U^T)^† = UH^{-φ}U^† = H^π ,
\]

we see that \(U^T\) is a symmetry of \(H^π\). It can be shown that \((UT)^2 = T^2 = −1\) (see App. [1]), so \(H^π\) also has a \(Z_2\) topological classification.

Considering the Hofstadter Hamiltonian as a 3D model with \(T\) symmetry, its topology is characterized by the magnetoelectric polarizability \(θ\). Ref. [25] demonstrates that \(θ\) is quantized by \(T\) to be 0 or \(π\), where \(π\) is the nontrivial value of the 3D TI phase, and that \(e^{iθ} = δ^{φ=0} × δ^{φ=π}\), where \(δ^{φ} \in \{−1, 1\}\) is the Pfaffian \(Z_2\) invariant protected by \(T\) (\(UT\)) at \(φ = 0\) (π) [20, 27]. Because we assume that the zero-field model is nontrivial, we need

\[3\]For pedagogical purposes, we assume that \(U\) is diagonal in momentum space. In the generic case, the algebra of \(UT\) and \(T_0(φ)\) acquires a projective phase which leads to an off-diagonal representation of \(UT\) on the magnetic BZ (see App. [7]).
only show that $\delta^{\phi=\pi} = +1$ in order to prove $\theta = \pi$. To do so, we introduce the parameter $M$ which tunes the $H^z$ to a trivial atomic limit as described in Sec. . Now consider the magnetic BZ at $\phi = \pi$ with $k_1 \in (-\pi, \pi), k_2 \in (0, \pi)$. The magnetic translation group requires the BZ to be $2\pi$ periodic, $\epsilon_m(k + \pi b_1) = \epsilon_m(k)$. As $M \to \infty$, we determine the change in $\delta^{\phi=\pi}$ by counting gap closings in half of the magnetic BZ [27][29]. For a gap closing at $k^*$, we choose the half to include the identical closing at $k^* + \pi b_1$. Each gap closing changes the sign of $\delta^{\phi=\pi}$, so it must be that $\delta^{\phi=\pi} = +1$ because an even number of gap closings occur between $M = 0$ and the trivial phase at $M = \infty$. We conclude $\theta = \pi$, proving that the Hofstadter Hamiltonian is a 3D TI. On open boundary conditions, such a model will pump gapless edge states into the bulk as $\phi$ is increased, as in exemplified in Fig. 1b. There, for a perturbed model with only $T$ symmetry $H^z_{QSH}$ (see App. F 1), we observe gapless edge states for small flux and their disappearance into the bulk.

We remark that the $\pi$ periodicity in the magnetic BZ was crucial to proving that $H^z$ is trivial. Generally, if the Hamiltonian is $\Phi = 2\pi n$ periodic in the flux, then the $U/T$-symmetric point exists at $\Phi/2 = n\pi$. When $n$ is odd, the BZ is still periodic under $k_1 \to k_1 + \pi$ allowing us to conclude that $\delta^{\phi=\pi} = +1$ (see App. D 2). However when $n$ is even, the BZ only has the usual $k_1 \to k_1 + 2\pi$ periodicity and our proof fails. Indeed, by adding a next-nearest neighbor hopping to $H_{QSH}$ and tuning the amplitude, we can build a model with $\Phi = 4\pi$ that realizes a weak TI phase with $\delta^{\phi=\pi} = -1$ or a 3D "strong" TI phase as we show in App. F 2.

IV. FRAGILE TOPOLOGICAL INSULATORS

The Hofstadter topological responses we have studied so far are those of phases which in zero flux are characterized by strong topological invariants: the Chern number, the Mirror Chern number, and the TRS-protected $Z_2$ index. We now study a fragile invariant: eigenvalue winding in the Wilson loop of 2 occupied bands protected by $C_{2z} T$ (with $(C_{2z} T)^2 = 1$) symmetry [8][30][31]. This winding number is $Z_2$ valued, but when more trivial bands are added, it is broken to a $Z_2$ classification, the second Stiefel-Whitney index $w_2$, a nontrivial value of which indicates fractional corner states [30][32][34]. The $w_2$ index may be computed from the Wilson loop eigenvalues, or the nested Wilson loop [30]. In 3D insulators, the HOTI phase is characterized by pumping corner states between a $w_2$ nontrivial phase and trivial phase [25][36]. Formally, this is indicated by the nontrivial value of the quantized magnetoelectric polarizability, $\theta = \pi$ [25]. Because $(C_{2z} T)^{-1} H^\phi \epsilon_m(C_{2z} T) = H^{-\phi} \epsilon_m(k)$, we can again identify $\phi$ with $k_2$ and classify the nontrivial Hofstadter topology as a 3D HOTI phase. We now develop the appropriate topological invariants to characterize this phase.

We have assumed that $C_{2z} T$ is a symmetry of $H^\phi_{\omega=0}$ and protects the invariant $w_2^\phi_{\omega=0}$. For a Hofstadter Hamiltonian that has a $\Phi = 2\pi n$ periodicity in flux, the other symmetric point occurs at $\phi = \Phi/2$ where $H^\Phi/2$ has the symmetry $UC_{2z} T$. Similarly to the TRS TI of Sec. , we can show that $(UC_{2z} T)^2 = \pm(C_{2z} T)^2$ where the sign must be calculated from the Peierls paths (see App. E 1). Different invariants describe the Hofstadter HOTI depending on this sign. If $(UC_{2z} T)^2 = +1$, a nonzero value of $\theta = \omega^\phi_{\phi=0} - \omega^\phi_{\phi=\pi}$ indicates corner state flow [30].

If $(UC_{2z} T)^2 = -1$, there is no $w_2$ index at $\phi = \pi$ [30]. However, we can diagnose the topology directly with the nested Wilson loop and Kramers’ theorem for $(UC_{2z} T)^2 = -1$ (see App. E 3), showing there are no

\[ \text{(c) The Wilson spectrum at } \phi = 3\pi \text{ is calculated in an extended } 2 \times 2 \text{ unit cell where } U \text{ is diagonal in momentum space (see App. G 3). Here, } w_2^\phi_{\omega=3\pi} = 0 \text{ because there are no crossings at } \vartheta = 0 \text{ and } \vartheta = \pi. \]

\[ \text{FIG. 2. (a) The Hofstadter Butterfly is calculated on a } 30 \times 30 \text{ lattice in the topological phase for } H^z_{TBC} \text{ which has only } C_{2z} T \text{ symmetry (see App. G 1). The corner modes are shown in red over the gapped black bulk and edge spectrum, and pump between the nontrivial } w_2 = 1 \text{ phase at } \phi = 0 \text{ to the trivial phase at } \phi = 3\pi \text{ where } w_2 = 0. \text{ This model is classified as a HOTI. (b) We observe from the Wilson loop spectrum, with eigenvalues exp i\theta(k_1), that } w_2^\phi_{\omega=0} = 1 \text{ due to the odd number of crossings at } \vartheta = 0 \text{ and } \vartheta = \pi. \text{ (c) The Wilson spectrum at } \phi = 3\pi \text{ is calculated in an extended } 2 \times 2 \text{ unit cell where } U \text{ is diagonal in momentum space (see App. G 3). Here, } w_2^\phi_{\omega=3\pi} = 0 \text{ because there are no crossings at } \vartheta = 0 \text{ and } \vartheta = \pi. \]

\[ \text{\footnote{The nontrivial phase with } \theta = \pi \text{ is a “strong” symmetry-protected topological phase with corner state pumping. If both } w_2^\phi_{\omega=0} = w_2^\phi_{\omega=\pi/2} = 1, \text{ then } \theta = 0 \text{ but both } H^\phi_{\omega=0} \text{ and } H^\phi_{\omega=\pi/2} \text{ have nontrivial corner states, which is a “weak” 3D fragile state.} } \]
protected corner states at $\phi = \Phi/2$ and the Hofstadter HOTI invariant depends only on the zero-field topology, i.e. $\theta^w = \theta^\Phi = 0$.

To exemplify the Hofstadter HOTI phase, we now consider a specific Hamiltonian $H_{TBG}$: a 4-band model of twisted bilayer graphene which possesses fragile Wilson loop winding yielding $w^\Phi_2 = 1$ [8, 37]. This model has the physical symmetries $C_{3z}, C_{2x}, C_{2z}, T$, as well as the accidental symmetries $C_{2z}$ and $T$ individually. We build a modified version $H_{TBG}$ (see App. G.1) that breaks $C_{2x}$ and $C_{3z}$ as well as the individual $C_{2z}, T$ symmetries leaving only $C_{2z}, T$ to protect the fragile topology. The Hofstadter Hamiltonian is $\Phi = 6\pi$ periodic in flux and has $(UC_{2z}T)^2 = +1$ (see App. G.1). In Fig. 2, we calculate the Hofstadter Butterfly on open boundary conditions and observe the pumping of corner modes (with a gapped bulk and edge) that characterizes a HOTI. We show that $\theta = \pi$ by calculating the $w_2$ indices at $\phi = 0, \Phi/2$ from the Wilson loop spectra shown in Fig. 2.b,c.

In fact, it is crucial that the $C_{2z}$ symmetry of $H_{TBG}$ be broken to realize the HOTI phase, which we show by constructing a modified Hamiltonian that preserves $C_{2z}$ and $T$ individually, but still breaks $C_{3z}$ and $C_{2x}$. For such a model, we prove (see App. G.4) that the Hofstadter Hamiltonian must have a bulk gap closing using the $C_{2z}$ eigenvalues. Similarly, the symmetry $C_{2z}T$ can protect a bulk gap closing which would also disrupt the appearance of the 3D HOTI phase (see App. G.5).

V. DISCUSSION

We have shown that the Hofstadter Hamiltonian exhibits a rich variety of higher dimensional topological phases in a mixed momentum-flux parameter space which extend the zero-field 2D topological phases. We demonstrated first that a nonzero Chern number or mirror Chern number enforces a bulk gap closing at the Fermi level in the Hofstadter Hamiltonian. In analogy to the 3D classifications, we call this a topologically protected Hofstadter semimetal. The Hofstadter topology of a Hamiltonian with a nontrivial $\mathbb{Z}_2$ index depended on the flux periodicity $\Phi = 2\pi n$. When $n$ is odd, we proved that the Hofstadter realized a 3D TI phase, but when $n$ is even, we showed by example that either a weak or strong TI phase was possible. Finally, we considered Hamiltonians with a nonzero $w_2$ index and found that the topological index of the Hofstadter HOTI phase depended the sign of $(UC_{2z}T)^2$, which is determined by the Peierls paths. We studied a model of twisted bilayer graphene and demonstrated that with only $C_{2z}T$ symmetry intact, the Hofstadter Hamiltonian realized the HOTI phase. In the era of Moiré lattices, we expect the results of this work to be experimentally verifiable in the near future [38, 40].

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Supplementary Appendices for "Hofstadter Topology: Non-crystalline Topological Materials in the Moiré Era"

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Appendix A: Features of the Hofstadter Hamiltonian

In this Appendix, we study Hofstadter Hamiltonian on an arbitrary lattice with arbitrary Peierls paths. We begin by discussing the Peierls substitution (App. A1). Then we prove the periodicity in flux and the gauge invariance of the Hofstadter Hamiltonian (App. A2). We derive the general form of the magnetic translation operators in App. A3. In the remainder of the section, we discuss the momentum space features of the Hofstadter Hamiltonian in a suitable Landau gauge \( \mathbf{A}(\mathbf{r}) = -\phi \mathbf{b}_1(\mathbf{r} \cdot \mathbf{b}_2) \). This choice of gauge is useful for numerical calculations of the spectrum, but has the disadvantage of generically requiring an enlarged magnetic unit cell that arises as an artifact of the gauge choice (Apps. A4 and A5). We discuss a residual \( SL(2,\mathbb{Z}) \) gauge symmetry associated with the Landau gauge in App. A6. We then construct the Hofstadter Hamiltonian in the Landau gauge (App. A7) and we give expressions for the embedding matrices which implement the periodicity in flux across the magnetic BZ (App. A8).

1. Peierls paths

To introduce a constant magnetic field to the lattice via the Peierls substitution, we must choose paths \( C_{r \rightarrow r'} \) connecting the orbitals at \( \mathbf{r} = \mathbf{R} + \mathbf{\delta}_\alpha, \mathbf{r}' = \mathbf{R}' + \mathbf{\delta}_\beta \) where \( \mathbf{R} = r_1 \mathbf{a}_1 + r_2 \mathbf{a}_2, \mathbf{R}' = r'_1 \mathbf{a}_1 + r'_2 \mathbf{a}_2 \) with \( r_1, r_2, r'_1, r'_2 \in \mathbb{Z} \) and \( \mathbf{\delta}_\alpha \) is the position of an orbital \( \alpha \) within the unit cell. Given a path, we calculate the Peierls phases,

\[
\varphi_{rr'} = \int_{C_{r \rightarrow r'}} \mathbf{A} \cdot d\mathbf{r},
\]

which modify the zero-field hoppings \( t_{\alpha \beta}(\mathbf{r} - \mathbf{r}') \rightarrow e^{i\varphi_{rr'}} t_{\alpha \beta}(\mathbf{r} - \mathbf{r}') \). Conventionally, the Peierls substitution is for nearest neighbors and consists of straight-line paths between the orbitals. Ref. [37] discusses Peierls’ approximation in more detail and demonstrated that the integral Eq. (A1) should be taken on piecewise straight paths from the orbitals through the points of greatest overlap of the local Wannier functions, possibly in superposition [22]. For instance, “s” \( \delta \)-function-like orbitals on sites should be connected by a straight-line path since they are centered on the atoms. In a more complicated example, our model of twisted bilayer graphene, the Wannier functions are extended and the paths are not straight but rather are taken through the center of the honeycomb [8, 37]. We show this in Fig. 3. We emphasize that the path \( C_{r \rightarrow r'} \) is physical; different paths lead to a different spectrum, resulting from the orbitals present in the model (see Ref. [37]). Of course, the additional gauge choice made in writing \( \mathbf{A} \) does affect the individual phases, but does not affect the spectrum.

2. Magnetic Periodicity and Gauge Invariance

A crucial feature of the Hofstadter Hamiltonian is its periodicity in the flux \( \phi \), which we anticipate because the flux dependence enters the Hofstadter Hamiltonian only as a phase. For simplicity, we work in units of length such that the unit cell area \( \mathbf{a}_1 \times \mathbf{a}_2 \) is set to 1. The flux periodicity is given by \( \Phi = 2\pi n, n \in \mathbb{N} \) such that taking \( \phi \rightarrow \phi + \Phi \) leaves the energy spectrum invariant. \( n \) is observable (in principle), gauge invariant, and exists so long as the Peierls
paths are commensurate, meaning that all loops along Peierls paths enclose a rational area (given \(a_1 \times a_2 = 1\)). As we will soon show, \(n\) is given by the least common denominator of the fractional area enclosed by all possible loops along the Peierls paths. For example, we consider the model of twisted bilayer graphene. Consulting the hoppings of the twisted bilayer graphene model in Fig. 3, we see all hoppings must pass through the center of the honeycomb and cannot go along the bonds. Examining the possible closed loops that can be constructed from the Peierls paths in Fig. 3, we see that all enclose multiples of 1/3 of a unit cell, so \(n = 3\).

We prove the periodicity of \(H^\Phi\) in flux by constructing the unitary transform \(U\) explicitly. Let \(A \rightarrow A + \tilde{A}\) where the flux of \(\tilde{A}\) through the unit cell, denoted \(\Omega\), is

\[
\nabla \times \tilde{A} = \Phi
\]

(recalling that we take the cross product of 2D vectors to be a scalar, and that the magnetic field is constant. The Peierls phases \(\varphi_{R \rightarrow \delta_a, R' \rightarrow \delta_b}\) acquire the additional contribution \(\int_{R \rightarrow \delta_a} \tilde{A} \cdot dr\). By the definition of \(n\), all closed line integrals of \(\tilde{A}\) which are taken along Peierls paths are pierced by an integer number of flux quanta. In what follows, we assume all integrals are taken along Peierls paths. Let \(r_0\) be an arbitrary but fixed orbital of the Hamiltonian that is connected by a sequence of Peierls paths to orbitals at \(R + \delta_a\) and \(R' + \delta_b\), and let \(C_{r_0}\) be a closed loop along Peierls paths connecting \(R + \delta_a, R' + \delta_b\), and \(r_0\) which we depict an example of in Fig. 3d. Then at \(\phi = \Phi\), we have

\[
\int_{C_{r_0}} \tilde{A} \cdot dr = \left( \int_{R \rightarrow \delta_a} + \int_{R' \rightarrow \delta_b} + \int_{r_0} \right) \tilde{A} \cdot dr = 0 \mod 2\pi
\]

from which we conclude

\[
\int_{R' \rightarrow \delta_b} \tilde{A} \cdot dr = \left( \int_{R \rightarrow \delta_a} + \int_{r_0} \right) \tilde{A} \cdot dr \mod 2\pi .
\]

This equation shows that the line integral of \(\tilde{A}\), generating \(\Phi\) flux, taken between two points \(R + \delta_a\) and \(R' + \delta_b\) along Peierls paths may be deformed to any other point \(r_0\) along Peierls paths without changing the value \(\mod 2\pi\). Because of this, whenever integrals in the form Eq. (A3) appear in exponentials, the integral is path independent as long as it is taken along Peierls paths. Now we construct the unitary transformation

\[
U^\dagger c_{R, \alpha} U = e^{i \int_{R \rightarrow \delta_a} \tilde{A} \cdot dr} c_{R' \alpha}, \quad U = \exp \left( i \sum_{R \rightarrow \delta_a} \int_{r_0} \tilde{A} \cdot dr \right) ,
\]

which acts on \(c_{R, \alpha}^\dagger\) (resp. \(c_{R, \alpha}\)), the fermion creation (resp. destruction) operator of the orbital \(\beta\) at \(R + \delta_a\). We note that the path of integration is arbitrary as long as it is taken along Peierls paths as per the prior discussion. Using the definition of \(U\), we compute

\[
U^\dagger H^\Phi U = U^\dagger \sum_{R \rightarrow \delta_a} \sum_{R' \rightarrow \delta_b} t_{\alpha \beta} (R + \delta_a - (R' + \delta_b)) e^{i \varphi_{R + \delta_a, R' + \delta_b} + \int_{R \rightarrow \delta_a} \tilde{A} \cdot dr} c_{R, \alpha}^\dagger U U c_{R', \beta} U
\]

\[
= \sum_{R \rightarrow \delta_a} \sum_{R' \rightarrow \delta_b} t_{\alpha \beta} (R + \delta_a - (R' + \delta_b)) e^{i \varphi_{R + \delta_a, R' + \delta_b} + \int_{R' \rightarrow \delta_b} \tilde{A} \cdot dr} c_{R, \alpha}^\dagger U U c_{R', \beta}
\]

\[
= \sum_{R \rightarrow \delta_a} \sum_{R' \rightarrow \delta_b} t_{\alpha \beta} (R + \delta_a - (R' + \delta_b)) e^{i \varphi_{R + \delta_a, R' + \delta_b} + \int_{r_0} \tilde{A} \cdot dr} c_{R, \alpha}^\dagger U U c_{R', \beta}
\]

\[
= \sum_{R \rightarrow \delta_a} \sum_{R' \rightarrow \delta_b} t_{\alpha \beta} (R + \delta_a - (R' + \delta_b)) e^{i \varphi_{R + \delta_a, R' + \delta_b} + \int_{r_0} \tilde{A} \cdot dr} \tilde{A} \cdot dr c_{R, \alpha}^\dagger c_{R', \beta}
\]

\[
= H^\Phi
\]

proving that the Hamiltonian is periodic in \(\Phi = 2\pi n\) up to a unitary transformation \(U\). We may think of \(U\) as a kind of “embedding matrix” in the flux direction, in analogy to the embedding matrix along \(k_z\) of 3D Bloch Hamiltonians [11].
path of integration in Eq. (A9) is taken to be a straight line between the 1a atoms separated by (0, 1) and also between neighboring 1a and 1b atoms separated by (1/2, 0). We take all Peierls paths to be straight lines between the atoms, so the paths are given by the lines shown in the figure. The smallest closed loop along Peierls paths encloses a single unit cell, and hence $n = 1$, $\Phi = 2\pi$. (b) We now allow the 1b atoms to be connected by a hopping of amplitude $t'$, shown by dotted lines. There is a closed loop that encloses half a unit cell (shaded in gray) by hopping between the 1b positions. In this case $n = 2$ and $\Phi = 4\pi$.

A very similar proof can be used to show that the Hofstadter Hamiltonian is also gauge-invariant with respect to the electromagnetic field up to a unitary transform. For clarity, we momentarily denote the Hamiltonian’s dependence on the gauge field as $H(A)$. If we change gauge to $A \to A + \nabla \lambda$, then we construct the new unitary transformation

$$\tilde{U} = \exp \left( i \sum_{R, \alpha} \lambda(R + \delta_{\alpha}) c_{R, \alpha}^\dagger c_{R, \alpha} \right)$$

(A7)

and calculate

$$\tilde{U}^\dagger H(A + \nabla \lambda) \tilde{U} = \tilde{U}^\dagger \sum_{RR'\alpha\beta} t_{\alpha\beta}(R - R') e^{i \varphi_{R+\delta_{\alpha}, R' + \delta_{\beta}} + i \int_{R' + \delta_{\beta}}^{R+\delta_{\alpha}} \nabla \lambda \cdot dr + i \int_{R' + \delta_{\beta}}^{R+\delta_{\alpha}} \delta_{\alpha}} - i \lambda(R' + \delta_{\beta}) \tilde{U}^\dagger c_{R, \alpha}^\dagger c_{R', \beta} \tilde{U}$$

(A8)

$$= \sum_{RR'\alpha\beta} t_{\alpha\beta}(R - R') e^{i \varphi_{R+\delta_{\alpha}, R' + \delta_{\beta}} + i \lambda(R + \delta_{\alpha}) - i \lambda(R' + \delta_{\beta})} \tilde{U}^\dagger c_{R, \alpha}^\dagger c_{R', \beta} \tilde{U}$$

$$= \sum_{RR'\alpha\beta} t_{\alpha\beta}(R - R') e^{i \varphi_{R+\delta_{\alpha}, R' + \delta_{\beta}} + i \lambda(R + \delta_{\alpha}) - i \lambda(R' + \delta_{\beta})} \tilde{U}^\dagger c_{R, \alpha}^\dagger c_{R', \beta} \tilde{U}$$

$$= H(A).$$

The transformation $\tilde{U}$ is the straightforward implementation of the $U(1)$ gauge symmetry of continuum electromagnetic to lattice fermions and is an important consistency check on the Peierls substitution.

We conclude this section with an example of a simple model with $n \neq 1$ (thus $\Phi \neq 2\pi$). Starting from the familiar square lattice Hofstadter model, we add atoms at the 1b position as shown in Fig. 4. If we connect the 1b sites with a hopping $t'$ taken along a straight-line Peierls path (shown with a dotted line in Fig. 4) then there is a closed loop along Peierls paths enclosing half a unit cell, so $n = 2$. Accordingly, shifting $\phi \to \phi + 2 \times 2\pi$ leaves the spectrum invariant and we identify $\Phi = 2\pi n = 4\pi$.

### 3. The Magnetic Translation Group

We now discuss the magnetic translation operators that commute with the Hamiltonian $H^\phi$ in the presence of flux. We will prove that the single-particle operators

$$T_i(\phi) = \sum_{R, \alpha} \exp \left( i \int_{R + \delta_{\alpha}}^{R+\delta_{\alpha} + a_i} A \cdot dr + i \chi_i(R + \delta_{\alpha}) \right) c_{R+\delta_{\alpha} + a_i, \alpha}^\dagger c_{R+\delta_{\alpha}, \alpha} |0\rangle \langle 0|_{C_{R, \alpha}}, \quad \chi_i(r) = \phi a_i \times r$$

(A9)

commute with $H^\phi$. We have inserted a projector $|0\rangle \langle 0|$ into Eq. (3) to arrive at Eq. (A9), which insures that $T_i^\dagger(\phi) = c_{R, \alpha}^\dagger T_i(\phi)$ is still a single-particle operator. Note that $T_i(\phi)$ is unitary on the single-particle Hilbert space. The path of integration in Eq. (A9) is taken to be a straight line between $R + \delta_{\alpha}$ and $R + a_i + \delta_{\alpha}$, although this is not
necessarily a Peierls path if the local Wannier functions are supported on the orbital sites and the Peierls path is not a straight line (see App. A1). We will prove \([T_1(\phi), H^\phi] = 0\) by showing \(T_1^\dagger(\phi)H^\phi T_1(\phi) = H^\phi\) in the single-particle Hilbert space. We expand the LHS to find

\[
T_1^\dagger(\phi)H^\phi T_1(\phi) = \sum_{R, \alpha, R', \beta} \exp \left( i \int_{R' + \delta_\beta}^{R + \delta_\alpha} A \cdot d\mathbf{r} - i \int_{R + \delta_\alpha}^{R + \delta_\alpha + a_i} A \cdot d\mathbf{r} - i \int_{R + \delta_\alpha}^{R + \delta_\alpha + a_i} A \cdot d\mathbf{r} - i \int_{R + \delta_\alpha}^{R + \delta_\alpha + a_i} A \cdot d\mathbf{r} + i\chi_i(R' + \delta_\beta) \right) 
\]

\[
\times t_{\alpha\beta}(R + \delta_\alpha, (R' + a_i + \delta_\alpha) + i\chi_i(R' + \delta_\beta) + i\chi_i(R' + \delta_\beta)) c_{R, \alpha} c_{R', \beta} 
\]

\[
= \sum_{R, \alpha, R', \beta} \exp \left( i \int_{R' + \delta_\beta}^{R + \delta_\beta} + \int_{R' + \delta_\beta}^{R + \delta_\beta} + \int_{R' + \delta_\beta}^{R + \delta_\beta} A \cdot d\mathbf{r} \right) 
\]

\[
\times t_{\alpha\beta}(R + \delta_\alpha, (R' + \delta_\beta) + i\chi_i(R' + \delta_\beta) + i\chi_i(R' + \delta_\beta)) c_{R, \alpha} c_{R', \beta} 
\]

\[
= \sum_{R, \alpha, R', \beta} \exp \left( i \int_{R' + \delta_\beta}^{R + \delta_\beta} + \int_{R' + \delta_\beta}^{R + \delta_\beta} + \int_{R' + \delta_\beta}^{R + \delta_\beta} A \cdot d\mathbf{r} \right) 
\]

\[
\times t_{\alpha\beta}(R + \delta_\alpha, (R' + \delta_\beta) + i\chi_i(R' + \delta_\beta) + i\chi_i(R' + \delta_\beta)) c_{R, \alpha} c_{R', \beta} 
\]

(A10)

The path of the open line integral (e.g. Fig. 5b) in Eq. (A10) can be rewritten as a closed path that doubles back on itself (e.g. Fig. 5b). Written out, we have

\[
\left( \int_{R' + \delta_\beta}^{R + \delta_\beta} + \int_{R' + \delta_\beta}^{R + \delta_\beta} + \int_{R' + \delta_\beta}^{R + \delta_\beta} \right) A \cdot d\mathbf{r} = \phi \int_{\mathcal{C}} A \cdot d\mathbf{r} = \phi \int_{\mathcal{R}} d\mathbf{S} = \phi (R' + \delta_\beta - (R + \delta_\alpha)) \times a_i 
\]

(A11)

where the closed loop \(\mathcal{C}\) (e.g. the boundary of the pink region in Fig. 5b) is formed from the straight-line paths \(R + \delta_\alpha + a_i \rightarrow R + \delta_\alpha\), \(R' + \delta_\beta \rightarrow R' + \delta_\beta + a_i\) of the magnetic translation operator and the Peierls path from \(R + \delta_\alpha + a_i \rightarrow R' + \delta_\beta + a_i\). In Fig. 5, the Peierls path shown in the example happens to be a straight-line path.

We now want to use Stokes’ theorem to reduce the closed line integral in Eq. (A11) to a surface integral over \(\mathcal{R}\), the area enclosed by \(\mathcal{C}\). \(\mathcal{R}\) is a polygon formed from two parallel sides of length \(a_i\) (corresponding to the straight-line paths of integration in the magnetic translation operator \(T_1(\phi)\) of Eq. (A9)) and two identical Peierls paths connecting the points \(R + \delta_\alpha\) and \(R' + \delta_\beta\) and the points \(R + \delta_\alpha + a_i\) and \(R' + \delta_\beta + a_i\), which we call \(\mathcal{P}_1\) and \(\mathcal{P}_2\) respectively. An example of such a region is shown in Fig. 4. If \(\mathcal{P}_1\) and \(\mathcal{P}_2\) were straight lines, then \(\mathcal{R}\) would be a parallelogram with area \((R' + \delta_\beta - (R + \delta_\alpha)) \times a_i\). In fact, \(\mathcal{R}\) still has area \((R' + \delta_\beta - (R + \delta_\alpha)) \times a_i\) for any (possibly piecewise-straight) Peierls path. This follows because any deviation in area due to \(\mathcal{P}_1\) not being straight and is canceled by the same deviation of \(\mathcal{P}_2\), as shown for example by the blue dashed lines in Fig. 4 for the Peierls paths of the twisted bilayer graphene model in App. G. Using this geometrical fact, we find that

\[
\phi \int_{\mathcal{C}} A \cdot d\mathbf{r} = \phi \int_{\mathcal{R}} d\mathbf{S} = \phi (R' + \delta_\beta - (R + \delta_\alpha)) \times a_i 
\]

(A12)
FIG. 6. We show an example of the area enclosed by the integral in Eq. (A12) for the Peierls paths of our model of twisted bilayer graphene (as shown in Fig. 5) and the magnetic translation operator \( T_2 \). The blue dashed lines are the Peierls’ paths \( \mathcal{P}_1 \) and \( \mathcal{P}_2 \) of the hoppings connecting the orbitals, and the red dashed lines show the path of integration in the \( T_2 \) operator (which is not generically a Peierls path). (a) We depict the area of the parallelogram formed by the vectors \((R + \delta_\alpha), (R + \delta_\beta), (R + a_2 + \delta_\alpha), (R + a_2 + \delta_\beta)\). (b) We depict the lattice vectors \( a_1 \). (c) We depict the lattice vectors \( a_1 \), the nearest-neighbor vectors \( \delta_\alpha \), and the third-nearest neighbor vectors \(-2\delta_1\).

We return to Eq. (A10) and using the results of Eqs. (A12) and (A11), we find

\[
T_i^\dagger(\phi) H^\phi T_i(\phi) = \sum_{R_\alpha, R_\beta} \exp \left( i \int_{R + \delta_\beta}^{R + \delta_\alpha} A \cdot dr + i\phi(R' + \delta_\beta - (R + \delta_\alpha)) \times a_i - i\chi_i(R + \delta_\alpha) + i\chi_i(R' + \delta_\beta) \right) \times t_{\alpha\beta}(R + \delta_\alpha - (R' + \delta_\beta)) c_{R,\alpha}^\dagger c_{R',\beta}.
\]

(A13)

Now we recall our choice of \( \chi_i(r) = \phi a_i \times r \) in Eq. (A9) and notice

\[
\phi(R' + \delta_\beta - (R + \delta_\alpha)) \times a_i - \chi_i(R + \delta_\alpha) + \chi_i(R' + \delta_\beta) = \phi(R' + \delta_\beta - (R + \delta_\alpha)) \times a_i + \phi a_i \times (R' + \delta_\beta - (R + \delta_\alpha)) = 0.
\]

(A14)

Hence, we find that Eq. (A13) simplifies to

\[
T_i^\dagger(\phi) H^\phi T_i(\phi) = \sum_{R_\alpha, R_\beta} \exp \left( i \int_{R + \delta_\beta}^{R + \delta_\alpha} A \cdot dr \right) t_{\alpha\beta}(R + \delta_\alpha - (R' + \delta_\beta)) c_{R,\alpha}^\dagger c_{R',\beta}
\]

(A15)

We have proven that the magnetic translation operators \( T_i(\phi) \) commute with \( H^\phi \) at all \( \phi \). To derive the magnetic translation group algebra, we start from Eq. (A9) and calculate

\[
T_1(\phi) T_2(\phi) = \sum_{R_\alpha} \exp \left( i \int_{R + \delta_\alpha + a_1 + a_2}^{R + \delta_\alpha + a_2} A \cdot dr + i\chi_1(R + a_2 + \delta_\alpha) + i \int_{R + \delta_\alpha}^{R + \delta_\alpha + a_2} A \cdot dr + i\chi_2(R + \delta_\alpha) \right) c_{R + a_1 + a_2}^\dagger c_{R,\alpha},
\]

\[
T_2(\phi) T_1(\phi) = \sum_{R_\alpha} \exp \left( i \int_{R + \delta_\alpha + a_1 + a_2}^{R + \delta_\alpha + a_1} A \cdot dr + i\chi_2(R + a_1 + \delta_\alpha) + i \int_{R + \delta_\alpha + a_1}^{R + \delta_\alpha + a_2} A \cdot dr + i\chi_1(R + \delta_\alpha) \right) c_{R + a_1 + a_2}^\dagger c_{R,\alpha},
\]

(A16)

which we use to find that, on the single-particle Hilbert space,

\[
(T_2(\phi) T_1(\phi))^\dagger T_1(\phi) T_2(\phi) = \sum_{R_\alpha} \exp \left[ i \int_{R + \delta_\alpha + a_1 + a_2}^{R + \delta_\alpha + a_2} A \cdot dr + i\chi_1(R + a_2 + \delta_\alpha) + i \int_{R + \delta_\alpha}^{R + \delta_\alpha + a_2} A \cdot dr + i\chi_2(R + \delta_\alpha) \right.
\]

\[
- i \int_{R + \delta_\alpha + a_1}^{R + \delta_\alpha + a_2} A \cdot dr - i\chi_2(R + a_1 + \delta_\alpha) - i \int_{R + \delta_\alpha + a_1}^{R + \delta_\alpha + a_2} A \cdot dr - i\chi_1(R + \delta_\alpha) \right]
\]

(A17)
Collecting the integrals, we see

\[
\begin{aligned}
\left(\int_{R+\delta_\alpha+a_1+a_2} & + \int_{R+\delta_\alpha+a_2} - \int_{R+\delta_\alpha+a_1} - \int_{R+\delta_\alpha}\right) \mathbf{A} \cdot d\mathbf{r} = -\phi \int_{\text{unit cell}} \mathbf{A} \cdot d\mathbf{r} \\
& = -\phi \int_{\text{unit cell}} dS
\end{aligned}
\]  

(A18)

where the minus sign has appeared because the path of integration is clockwise, and we recall that the area of the unit cell is one. Collecting the \(\chi_i\) terms from Eq. (A17), we find

\[
\chi_1(R + a_2 + \delta_\alpha) + \chi_2(R + \delta_\alpha) - \chi_2(R + a_1 + \delta_\alpha) - \chi_1(R + \delta_\alpha) = \phi a_1 \times (R + a_2 + \delta_\alpha - (R + \delta_\alpha))
\]

\[
+ \phi a_2 \times (R + \delta_\alpha - (R + a_1 + \delta_\alpha))
\]

\[
= \phi a_1 \times a_2 - \phi a_2 \times a_1
\]

\[
= 2\phi a_1 \times a_2
\]

\[
= 2\phi
\]

(A19)

because we have normalized the unit cell to be \(a_1 \times a_2 = 1\). Using the results of Eqs. (A18) and (A19), we return to Eq. (A17) and find

\[
(T_2(\phi)T_1(\phi))^\dagger T_1(\phi)T_2(\phi) = \sum_{R_\alpha} e^{-i\phi + 2i\phi} c_{R_\alpha}^\dagger c_{R_\alpha} = e^{i\phi}
\]

(A20)

recalling that \(\sum_{R_\alpha} c_{R_\alpha}^\dagger c_{R_\alpha} = 1\) when acting on single particle states. Eq. (A20) is the usual single-particle algebra of the magnetic translation operators.

4. Peierls Phases

So far, we have discussed the magnetic translation group in position space which demonstrates the existence of a \(1 \times q\) magnetic unit cell at \(\phi = \frac{2\pi p}{q}\), \(p, q\) coprime. We now discuss a particular gauge choice, a certain Landau gauge, that will makes explicit calculations in momentum space tractable. We work in the Landau gauge \(\mathbf{A}(\mathbf{r}) = -\phi \mathbf{b}_1(\mathbf{r} \cdot \mathbf{b}_2)\) which obeys

\[
\nabla \times \mathbf{A}(\mathbf{r}) = -\phi \mathbf{b}_2 \times \mathbf{b}_1 = \phi
\]

(A21)

where we have used that \(\mathbf{b}_1 \times \mathbf{b}_2 = a_1 \times a_2 = 1\). This choice of gauge is practical. We will see that the Peierls phases do not depend on \(r_1\), the coordinate along \(a_1\), so the unit cell of the Hofstadter Hamiltonian is only extended along one direction. Thus we may Fourier transform along \(a_1\) and obtain an effective 1D chain along \(a_2\) which is not a priori periodic because of the dependence on \(r_2\). However, for a certain choice of rational flux (in this specific gauge choice), an extended spatial periodicity reappears and enables the Hamiltonian to be Fourier transformed into momentum space. Importantly, at \(\phi = \frac{2\pi p}{q}\), \(p, q\) coprime, the Landau gauge does not permit a \(1 \times q\) unit cell on a general lattice, and may need to be enlarged to a \(1 \times q'\) unit cell for \(q' > q\). We will discuss this extensively in App. A.5 In App. D.2 we introduce a gauge-invariant formalism where the minimal \(1 \times q\) magnetic unit cell is manifest. However, the Landau gauge is a much more convenient choice for numerical calculations because we can derive explicit expressions for the Peierls phases.

First we show that in our Landau gauge, all Peierls phases (Eq. (A11)) must be of the form \(\varphi_{\mathbf{r},\mathbf{r}'} = \phi (\rho_{\mathbf{r},\mathbf{r}'} r_2 + \rho'_{\mathbf{r},\mathbf{r}'} r_2')\) with \(\rho_{\mathbf{r},\mathbf{r}'} \in \mathbb{Q}\) so long as the orbitals are commensurate, meaning that \(\mathbf{R}' + \delta_\beta - (\mathbf{R} + \delta_\alpha)\) is a rational linear combination of the lattice vectors. As an example of an incommensurate orbitals, consider a lattice with atoms at the positions \(x_1, \ldots, x_N\) (noting that the beginning and ending points are \(x_1 = \mathbf{R} + \delta_\alpha\) and \(x_N = \mathbf{R}' + \delta_\beta\) respectively). We now calculate the Peierls phase accumulated along the path \(\mathcal{C}\). Breaking up the integral Eq. (A1) along the piecewise-straight path, we find

\[
\varphi_{x_1; x_N} = \int_{\mathcal{C}} \mathbf{A} \cdot d\mathbf{r} = \sum_{i=1}^{N-1} \int_{x_i}^{x_{i+1}} \mathbf{A} \cdot d\mathbf{r}.
\]

(A22)
We compute
\[
\int_{\mathbf{x}_i}^{\mathbf{x}_{i+1}} \mathbf{A} \cdot d\mathbf{r} = -\phi \int_0^1 \mathbf{b}_2 \cdot (\mathbf{x}_i + t(\mathbf{x}_{i+1} - \mathbf{x}_i)) \mathbf{b}_1 \cdot (\mathbf{x}_{i+1} - \mathbf{x}_i) dt
\]
\[
= -\phi \mathbf{b}_1 \cdot (\mathbf{x}_{i+1} - \mathbf{x}_i) \int_0^1 (\mathbf{b}_2 \cdot \mathbf{x}_i + t\mathbf{b}_2 \cdot (\mathbf{x}_{i+1} - \mathbf{x}_i)) dt
\]
\[
= -\phi \mathbf{b}_1 \cdot (\mathbf{x}_{i+1} - \mathbf{x}_i) \left( \mathbf{b}_2 \cdot \mathbf{x}_i + \frac{1}{2} \mathbf{b}_2 \cdot (\mathbf{x}_{i+1} - \mathbf{x}_i) \right)
\]
\[
= -\phi \frac{1}{2} \mathbf{b}_1 \cdot (\mathbf{x}_{i+1} - \mathbf{x}_i) \left( \mathbf{b}_2 \cdot (\mathbf{x}_{i+1} + \mathbf{x}_i) \right).
\]

We work with a fixed reference point ("origin") at \( r_1 \mathbf{a}_1 + r_2 \mathbf{a}_2 \), \( r_1, r_2 \in \mathbb{Z} \) and define \( \mathbf{t}_i = \mathbf{x}_i - (r_1 \mathbf{a}_1 + r_2 \mathbf{a}_2) \). Note that because the \( \mathbf{x}_i \) are assumed commensurate, each \( \mathbf{t}_i \) is also commensurate. Then we have
\[
\int_{\mathbf{x}_i}^{\mathbf{x}_{i+1}} \mathbf{A} \cdot d\mathbf{r} = -\phi \mathbf{b}_1 \cdot (\mathbf{t}_{i+1} - \mathbf{t}_i) \left( \mathbf{b}_2 \cdot (r_1 \mathbf{a}_1 + r_2 \mathbf{a}_2 + \frac{1}{2}(\mathbf{t}_{i+1} + \mathbf{t}_i)) \right)
\]
\[
= -\phi \mathbf{b}_1 \cdot (\mathbf{t}_{i+1} - \mathbf{t}_i) \left( \mathbf{r}_2 + \frac{\mathbf{b}_2}{2} \cdot (\mathbf{t}_{i+1} + \mathbf{t}_i) \right)
\]
using \( \mathbf{a}_i \cdot \mathbf{b}_2 = \delta_{i2} \). Then by Eq. (A22), we find
\[
\varphi_{\mathbf{x}_i \mathbf{x}_N} = -\phi \sum_{i=1}^{N-1} \mathbf{b}_1 \cdot (\mathbf{t}_{i+1} - \mathbf{t}_i) \left( \mathbf{r}_2 + \frac{\mathbf{b}_2}{2} \cdot (\mathbf{t}_{i+1} + \mathbf{t}_i) \right)
\]
\[
= -\phi \mathbf{r}_2 \left[ \mathbf{b}_1 \cdot \sum_{i=1}^{N-1} (\mathbf{t}_{i+1} - \mathbf{t}_i) \right] - \phi \left[ \sum_{i=1}^{N-1} \mathbf{b}_1 \cdot (\mathbf{t}_{i+1} - \mathbf{t}_i) \left( \frac{\mathbf{b}_2}{2} \cdot (\mathbf{t}_{i+1} + \mathbf{t}_i) \right) \right]
\]

We recognize
\[
\rho_{\mathbf{r}\mathbf{r}'} = -\sum_{i=1}^{N-1} \mathbf{b}_1 \cdot (\mathbf{t}_{i+1} - \mathbf{t}_i), \quad \rho'_{\mathbf{r}\mathbf{r}'} = -\sum_{i=1}^{N-1} \mathbf{b}_1 \cdot (\mathbf{t}_{i+1} - \mathbf{t}_i) \left( \frac{\mathbf{b}_2}{2} \cdot (\mathbf{t}_{i+1} + \mathbf{t}_i) \right)
\]

Additionally, we observe that our expression for \( \rho_{\mathbf{r}\mathbf{r}'} \) can be simplified because the sum telescopes, canceling term by term:
\[
\rho_{\mathbf{r}\mathbf{r}'} = -\sum_{i=1}^{N-1} \mathbf{b}_1 \cdot (\mathbf{t}_{i+1} - \mathbf{t}_i)
\]
\[
= -\mathbf{b}_1 \cdot (\mathbf{t}_N - \mathbf{t}_1)
\]
\[
= -\mathbf{b}_1 \cdot (r_1 \mathbf{a}_1 + r_2 \mathbf{a}_2 + \mathbf{t}_N - (r_1 \mathbf{a}_1 + r_2 \mathbf{a}_2 + \mathbf{t}_1))
\]
\[
= -\mathbf{b}_1 \cdot ((\mathbf{R} + \mathbf{\delta}_o) - (\mathbf{R}' + \mathbf{\delta}_o))
\]
and hence \( \rho_{\mathbf{r}\mathbf{r}'} \) is rational because \( \mathbf{b}_1 \cdot \mathbf{a}_i = \delta_{i1} \) and \( (\mathbf{R}+\mathbf{\delta}_o) - (\mathbf{R}'+\mathbf{\delta}_o) \) is assumed to be a rational linear combination of the lattice vectors because the orbitals are commensurate. Eq. (A27) will be useful as we now determine the magnetic unit cell. We emphasize that the Peierls phases are calculated on open paths and hence are gauge-dependent.

### 5. Rationalization of the Flux

In this section we will demonstrate how to determine the magnetic unit cell in the Landau gauge at rational values of the flux \( \phi \). We begin by recalling the well-known procedure on the square lattice. When the Peierls paths are taken along the bonds in the Landau gauge \( A(r) = -\phi(y,0) \), only the \( x \)-directed hoppings acquire nontrivial Peierls phases such that the hopping term becomes \( e^{-\phi(x)} c_{x+1,y}^c c_{x,y} \). For \( \phi \neq 0 \), the unit cell is broken. However, we can recover a \( 1 \times q \) unit cell where \( y \rightarrow y + q \) leaves all the Peierls phases invariant when \( \phi \) takes the values \( \phi = \frac{2\pi p}{q} \), \( p, q \) coprime. We emphasize that this specific magnetic unit cell derives from our Landau gauge choice. Because we can find \( p, q \) such that \( \phi \) is arbitrarily close to any real number, we are able to form the Hofstadter Hamiltonian in
hence prove that we must rationalize the flux to be \( \phi \). The Peierls phases are not generally periodic in the \( 1 \times q \) magnetic unit cell. In our Landau gauge, all Peierls phases are in the form \( \varphi_{\tau\tau'} = \phi(\rho_{\tau\tau'}(r_2 + q')) / q' \) (Eq. A26). Under a translation by \( T_2^q \) which amounts to taking \( r_2 \rightarrow r_2 + q \), we have \( \varphi_{\tau\tau'} \rightarrow \varphi_{\tau\tau'} + 2\pi p \rho_{\tau\tau'} \) with \( \phi = 2\pi p/q \). Generically, \( p \rho_{\tau\tau'} \) is not an integer and hence the Peierls phase is not periodic in the \( 1 \times q \) magnetic unit cell. We now show that the Peierls phases are periodic for our gauge choice over a \( 1 \times q' \) magnetic unit cell with \( q' \geq q \) if the flux is rationalized to be \( \phi = \frac{2\pi p}{q} \) where \( \mu \in \mathbb{N} \) depends on the orbital positions and the choice of Landau gauge. (Note that \( \mu \) depends on the gauge and is unrelated to \( n \) and the flux periodicity \( \Phi = 2\pi n \).)

Now we give an expression for \( \mu \) in the Landau gauge. Let \( \mu \in \mathbb{N} \) be the least common denominator (lcd) — equivalently the greatest common factor of the denominators — of \( \{\rho_{\tau\tau'}\} \) for each hopping of the model. Because \( \mathbf{R} \) and \( \mathbf{R}' \) are lattice vectors and \( \mathbf{b}_1 \cdot \mathbf{a}_i = \delta_{i1}, \mathbf{b}_1 \cdot (\mathbf{R} - \mathbf{R}') \) is an integer, the rational part of \( \rho_{\tau\tau'} \) is \( -\mathbf{b}_1 \cdot (\delta_\alpha - \delta_\beta) \) and hence

\[
\mu = \text{lcd} \{ \mathbf{b}_1 \cdot (\delta_\beta - \delta_\alpha) \} \text{ for all hoppings connecting } \mathbf{R} + \delta_\alpha \text{ and } \mathbf{R}' + \delta_\beta .
\]  

(A28)

We seek to determine what (rational) value of the flux \( \phi \) permits a spatial periodicity in the Peierls phases Eq. A25 along \( r_2 \). For a \( 1 \times q' \) unit cell, meaning that all Peierls phases at \( r_2 \) and \( r_2 + q' \) are identical modulo \( 2\pi \), we will prove that we must rationalize the flux to be

\[
\phi = \frac{2\pi p'}{q'}, \quad p', q' \in \mathbb{Z}, \text{ coprime} .
\]  

(A29)

We see that the minimal \( 1 \times q \) magnetic unit cell at \( \phi = \frac{2\pi p}{q} \) given by the magnetic translation group does not generically coincide with the \( 1 \times q' \) magnetic unit cell which results from choosing the Landau gauge. Throughout this section, we define \( p' \) and \( q' \) by \( p/q = \mu p'/q' \) with \( \mu \) fixed by Eq. A29 at \( \phi = \frac{2\pi p}{q} \). Note that \( q \) and \( q' \) are related by \( q = q' \cdot \text{gcd}(q, \mu) \) so \( q' \) is an integer multiple of \( q \) and \( q' \geq q \).

In the \( 1 \times q' \) magnetic unit cell, the Peierls phases are periodic and we can diagonalize the Hofstadter Hamiltonian in momentum space. The \( 1 \times q' \) unit cell is more convenient for practical purposes, such as determining the spectrum numerically. We emphasize that \( \mu \), and hence the magnetic unit cell defined by \( q' \), are both gauge-dependent. It is only the quantity \( \mu p'/q' = \phi/(2\pi) \) that is gauge-invariant.

We prove Eq. A29 now. For brevity, we denote the Peierls phases \( \varphi_{\mathbf{R} + \delta_\alpha, \mathbf{R}' + \delta_\beta} \) as \( \varphi_{\tau_2,\tau_1' \alpha, \beta} \), recalling that \( \mathbf{R} = r_1 \mathbf{a}_1 + r_2 \mathbf{a}_2 \) is the reference point as in Eq. A25 and \( \mathbf{R}' = r_1' \mathbf{a}_1 + r_2' \mathbf{a}_2 \) is the unit cell of the second orbital. We have used Eq. A25 to show that \( \varphi_{\mathbf{R} + \delta_\alpha, \mathbf{R}' + \delta_\beta} \) does not depend on \( r_1 \). Then we have, under \( r_2 \rightarrow r_2 + q' \),

\[
\varphi_{\tau_2,\tau_1' \alpha, \beta} = (\rho_{\tau\tau'}(r_2 + q') + \rho_{\tau\tau'}) \phi = \varphi_{\tau_2,\tau_1' \alpha, \beta} + \mu \frac{2\pi p'}{q'} \rho_{\tau\tau'}
\]

(A30)

Thus \( \varphi_{\tau_2,\tau_1' \alpha, \beta} \) only depends on \( r_2 \mod q' \), showing that the Peierls paths, and hence the Hofstadter Hamiltonian, has a \( 1 \times q' \) unit cell. In many simple examples of the Hofstadter Butterfly [1, 42], the orbitals are all on the atomic sites, so \( \delta_\alpha = 0 \) for all \( \alpha \). In this case, Eq. A28 trivially gives \( \mu = 1 \), and the flux takes the familiar form \( \phi = \frac{2\pi p'}{q'} = \frac{2\pi p}{q} \), so \( p = p' \) and \( q = q' \).

We now turn to the example of the square lattice with 1b atoms (see Fig. 4) to discuss \( \mu \neq 1 \). If we choose the lattice vectors \( \mathbf{a}_1 = (1, 0), \mathbf{a}_2 = (0, 1) \) (noting \( \mathbf{a}_1 \times \mathbf{a}_2 = +1 \)), then \( \mathbf{b}_1 = (1, 0) \). We calculate \( \mu \) using Eq. A28 and find

\[
\mu = \text{lcd} \{ \mathbf{b}_1 \cdot (0, 0), \mathbf{b}_1 \cdot (1/2, 0), \mathbf{b}_1 \cdot (0, 0) \}
\]

\[
= \text{lcd} \{ (1, 0) \cdot (0, 0), (1, 0) \cdot (1/2, 0), (1, 0) \cdot (0, 0) \}
\]

(A31)

This means that at \( \phi = \frac{2\pi p'}{q'} \), we can Fourier transform in the Landau gauge over a \( 1 \times q' \) unit cell. Note that \( \mu = 2 \) even when the \( t' \) hopping is zero, since it arises from the hopping connecting the 1a and 1b atoms (see Fig. 4). Thus we
see that when \( t' = 0 \) we have \( n = 1, \mu = 2 \) and when \( t' \neq 0 \) we have \( n = 2, \mu = 2 \) in this gauge. Alternatively, we could choose a different Landau gauge \( A'(r) = -\phi b'(r \cdot b') \) given by \( a'_1 = (0, 1), a'_2 = (-1, 0) \) (noting \( a'_1 \times a'_2 = +1 \)) where \( b'_1 = (0, 1) \). In this gauge, we compute

\[
\mu' = \text{lcd} \{b'_1 \cdot (0, 0), b'_1 \cdot (1/2, 0), b'_1 \cdot (0, 0)\} = \text{lcd} \{(0, 1) \cdot (0, 0), (0, 1) \cdot (1/2, 0), (0, 1) \cdot (0, 0)\} = 1.
\]

Again, this result does not depend on \( t' \). Hence in this gauge we have \( n = 1, \mu' = 1 \) when \( t' = 0 \) and \( n = 2, \mu' = 1 \) when \( t' \neq 0 \). The values of \( \mu \) are distinct in the different gauges, but \( n \) is the same. Indeed, \( \Phi = 2\pi n \) is gauge-invariant, whereas \( \mu \) simply allowed us to Fourier transform the Peierls phases in a given gauge.

In some cases (but not all), it is possible to choose lattice vectors so that the Landau gauge \( A(r) = -\phi b_1 (r \cdot b_2) \) yields \( \mu = 1 \), which we discuss now.

6. Residual \( SL(2, Z) \) Gauge Freedom

Despite fixing our gauge to the Landau gauge \( A(r) = -\phi b_1 (r \cdot b_2) \) which ensures a \( 1 \times q' \) magnetic unit cell, there is a residual gauge freedom which arises due to the choice of reciprocal lattice vectors \( b_i \). In deriving Eq. (A28), the form of the Peierls phases which defines \( \mu \) (Eq. (A28)), we relied on the fact that \( b_i \cdot a_j = \delta_{ij} \). For any given set of basis vectors \( a_i, b_i \), it is defined uniquely and our Landau gauge is fixed. However, we can gauge transform to a different Landau gauge \( A'(r) = -\phi b'_1 (r \cdot b'_2) \) while preserving the form of Eq. (A28) by choosing new lattice vectors

\[
a'_1 = m_{11} a_1 + m_{12} a_2, \quad m_{ij} \in \mathbb{Z}.
\]

For \( a'_1 \) to preserve the area of the unit cell, we require \( a'_1 \times a'_2 = b'_1 \times b'_2 = 1 \) which holds iff \( \text{det}[m] = m_{11} m_{22} - m_{12} m_{21} = 1 \). Thus \( [m] \in SL(2, \mathbb{Z}) \). The corresponding reciprocal lattice is spanned by \( b'_i \) satisfying \( b'_i \cdot a'_j = \delta_{ij} \) and \( \nabla \times A'(r) = \phi b'_1 \times b'_2 = \phi \). It can be checked using \( \text{det}[m] = 1 \) that the reciprocal vectors are given by

\[
b'_1 = m_{22} b_1 - m_{21} b_2, \quad b'_2 = -m_{12} b_1 + m_{11} b_2.
\]

We find that even after fixing the form of our Landau gauge, there is still a nontrivial residual gauge symmetry

\[
A'(r) = -\phi b'_1 (r \cdot b'_2) = A(r) + \nabla \Lambda
\]

where one may verify that \( \Lambda = \frac{\phi}{\pi} \left( (r \cdot b_1)(r \cdot b_2) - (r \cdot b'_1)(r \cdot b'_2) \right) \) by direct computation. In the gauge \( A'(r) \), we find a new rationalization of the flux \( \phi = \mu' \frac{2\pi n}{q' q''} \) where

\[
\mu' = \text{lcd} \{b'_1 \cdot (\delta_\beta - \delta_\alpha)\} \quad \text{for all hoppings connecting } R + \delta_\alpha \text{ and } R' + \delta_\beta.
\]

This is once again an illustration that \( \mu \) is gauge-dependent. It is tempting to think that with an appropriate \( SL(2, \mathbb{Z}) \) gauge transformation, it is possible to find a basis where \( \mu' = 1 \). We prove a condition on the orbitals \( \delta_\alpha \), demonstrating when it is possible to find such a basis, but we also show that in general it is impossible, i.e. that there is no choice of basis where \( \mu = 1 \) in our Landau gauge.

\( \mu \) is calculated from the distances between hoppings \( \{\delta_\beta - \delta_\alpha\} \). Because we assume \( \delta_\beta - \delta_\alpha \) is a rational sum of lattice vectors, we have \( \delta_\beta - \delta_\alpha = \omega_{1,\alpha,\beta} a_1 + \omega_{2,\alpha,\beta} a_2 \) for \( \omega_{1,\alpha,\beta}, \omega_{2,\alpha,\beta} \in \mathbb{Q} \). By Eq. (A28), we have

\[
\mu' = \text{lcd} \{b'_1 \cdot (\omega_{1,\alpha,\beta} a_1 + \omega_{2,\alpha,\beta} a_2)\} \quad \text{for all hoppings connecting } R + \delta_\alpha \text{ and } R' + \delta_\beta.
\]

Let \( \mu = \text{lcd} \{\omega_{i,\alpha,\beta}\} \) for all hoppings connecting \( R + \delta_\alpha \) and \( R' + \delta_\beta \). If \( \mu_1 \) and \( \mu_2 \) are coprime, it is possible to set \( \mu' = 1 \). We show this by explicitly constructing \( [m] \). Set \( m_{22} = \mu_1 \) and \( m_{21} = -\mu_2 \) in which case \( m_{22} \omega_{1i} = \mu_1 \omega_{1i} \in \mathbb{Z} \) and \( -m_{21} \omega_{2i} = \mu_2 \omega_{2i} \in \mathbb{Z} \) for all \( i \). Hence \( \mu' = 1 \). Additionally, there exist \( m_{11}, m_{12} \in \mathbb{Z} \) such that \( \text{det}[m] = \mu_1 m_{11} + \mu_2 m_{12} = 1 \). Indeed, \( \mu_1 \) and \( \mu_2 \) are coprime. We can thus choose \( m_{12} \) to be the modular inverse of \( \mu_2 \), i.e. \( \mu_2 m_{12} = 1 \mod \mu_1 \), simultaneously setting \( m_{11} \in \mathbb{Z} \) such that \( \mu_2 m_{12} = 1 - m_{11} \mu_1 \).

However, when \( \mu_1 \) and \( \mu_2 \) are not coprime, this proof fails. We now give an example of such a case where it is impossible to construct a basis where \( \mu = 1 \). Let there be three orbitals \( \delta_1 = (0, 0), (1/2, 1/2), (1/2, 1/4) \) in the
The Hamiltonian can be written in terms of these operators \( N_r \) and diagonalize magnetic unit cell. From the magnetic translation group, we know that it is possible to make a gauge transformation \( N_{\alpha} \) with positions \( a_\mu \) for a general \( \mu \) that there exist lattices where it is impossible to find such a basis. In the remaining sections, we develop our theory of the \( \phi \) vectors. We gave a simple criterion to determine if it is generically possible to find a basis such that \( m_{22} = m_{21} + 2s, s \in \mathbb{Z} \). Then

\[
\frac{1}{4}(2m_{22} - m_{21}) = \frac{1}{4}(m_{21} + 4s)
\]

is an integer only if \( m_{21} \) is a multiple of 4. But \( m_{22} - m_{21} \in 2\mathbb{Z} \) implies \( m_{21} \) is then a multiple of 2, so \( m_{21} \) and \( m_{22} \) are not coprime.

In summary, we have shown that at \( \phi = \frac{2n\pi}{q} = \mu \frac{2\pi q'}{q} \) for \( p', q' \) coprime, the Peierls phases are periodic in a \( 1 \times q' \) magnetic unit cell in our Landau gauge. \( \mu \) is calculated from the positions of the orbitals and the choice of lattice indices because it is useful to think of them in a tensor product basis. We have shown that at \( \phi = \frac{2n\pi}{q} \) the Peierls phases are periodic over the magnetic lattice, we have \( \phi \) and the magnetic BZ is defined as

\[
\begin{align*}
\sum_{r_2} e^{-i\phi(r_1a_1 + r_2 a_2 + (\alpha + \delta_\alpha a_\mu + \delta_\beta))} c_{k_1,r_1,\ell,\alpha}^\dagger c_{k_2,r_2,\ell,\beta} \\
= \sum_{k_1,k_2} \sum_{\ell,\alpha,\ell,\beta} c_{k_1,k_2,\ell,\alpha,\ell,\beta} c_{k_1,k_2,\ell,\alpha,\ell,\beta} \mathcal{H}(k_1,k_2) \mathcal{H}(k_1,k_2)^\dagger
\end{align*}
\]

where \( \mathcal{H} \) is the Fourier transform over the magnetic lattice:

\[
\mathcal{H}(k_1,k_2)_{\ell,\alpha,\ell,\beta} = \frac{1}{N/|q'|} \sum_{r_1,r_1',r_2} e^{i\phi(\alpha,\ell,\beta)} (r_1 - r_1') \mathcal{H}(k_1,k_2)_{\ell,\alpha,\ell,\beta} c_{k_1,k_2,\ell,\alpha}^\dagger c_{k_1,k_2,\ell,\beta} \\
\times t_{\alpha,\beta}(r_1 - r_1') (r_2 - r_2') q' a_2 + (\ell - \ell') a_2 + (\delta_\alpha - \delta_\beta)
\]

and the magnetic BZ is defined as \( k_1 = \frac{2n\pi}{N_1}(0, \ldots, N_x - 1) \), \( k_2 = \frac{2n\pi}{N_2}(0, \ldots, N_y/q' - 1) \). We note that for an infinite crystal, i.e. taking \( N_1, N_2 \to \infty \), the magnetic BZ is defined to be \( k_1 \in (-\pi, \pi), k_2 \in (0,2\pi/q') \). At a given momentum, the matrix Eq. (A42) can be diagonalized numerically to determine the \( q' n_{\text{orb}} \) band energies. We have separated the \( \ell, \alpha \) indices because it is useful to think of them in a tensor product basis.

7. Construction of the Hofstadter Hamiltonian

We have shown that our choice of Landau gauge preserves translation invariance along \( a_1 \), but at \( \phi = \mu \frac{2n\pi}{q} \), there is only translational invariance along \( a_1 \) given by \( r_2 \to r_2 + q' \) even if \( \mu \) and \( q' \) are not coprime. By choosing the Landau gauge, we are able to easily calculate the Peierls phases and form the Hofstadter Hamiltonian in a \( 1 \times q' \) magnetic unit cell. From the magnetic translation group, we know that it is possible to make a gauge transformation and diagonalize \( H^\phi \) in the minimal \( 1 \times 1 \) unit cell at \( \phi = \frac{2n\pi}{q} \), but it is difficult to find such a gauge explicitly. The Landau gauge is much more convenient for numerics, even at the cost of a larger magnetic unit cell.

Redefining \( r_1 \) and \( r_2 \), we write an atomic position in the crystal in the form \( r_1 a_1 + q' r_2 a_2 + (a_2 + \delta_\beta) \) where \( \ell = 0, \ldots, q' - 1 \) indexes the zero-field unit cells within the magnetic unit cell, and the orbitals are given by \( \alpha = 1, \ldots, N_{\text{orb}} \) with positions \( \delta_\alpha \). Because the Peierls phases are periodic over the magnetic lattice, we have

\[
\varphi^\ell r_1,\ell,\alpha,\ell,\beta = \varphi^\ell r_1,\ell,\beta
\]

The momentum space operators are defined as usual in the magnetic unit cell. In this notation, they are given by

\[
\begin{align*}
c_{k_1,k_2,\ell,\alpha}^\dagger &= \frac{1}{\sqrt{N/|q'|}} \sum_{r_1,r_2} e^{-i\phi(\alpha,\ell,\beta)} (r_1, r_1') a_1 + (r_2 - r_2') q' a_2 + (\ell - \ell') a_2 + (\delta_\alpha - \delta_\beta)) c_{k_1,k_2,\ell,\alpha}^\dagger c_{k_1,k_2,\ell,\beta} \\
&= \sum_{k_1,k_2} \sum_{\ell,\alpha,\ell,\beta} c_{k_1,k_2,\ell,\alpha,\ell,\beta} c_{k_1,k_2,\ell,\alpha,\ell,\beta} \mathcal{H}(k_1,k_2)_{\ell,\alpha,\ell,\beta} c_{k_1,k_2,\ell,\alpha}^\dagger c_{k_1,k_2,\ell,\beta}
\end{align*}
\]
We comment now on the apparent discontinuity that $\mathcal{H}^\phi(k)$ suffers. Because commuting translation operators only exist when $\phi$ is rational, $\mathcal{H}^\phi(k)$ only exists at $\phi = \frac{2\pi p}{q'}$. Additionally, the Fourier transform is only well-defined when the number of lattice sites (on periodic boundary conditions as we have assumed) is a multiple of $q'$. For two arbitrarily close values of $\phi$, their denominators may be arbitrarily different, and for any finite size lattice, $\mathcal{H}^\phi(k)$ may not strictly exist. While $\mathcal{H}$ and $k$ have very discontinuous behavior in $\phi$, the spectrum of $\mathcal{H}^\phi$ evolves smoothly. Ref. [1] proves that the spectrum is continuous for the simple Hamiltonian which it considers, but extending this proof to momentum space for a general Hamiltonian is beyond the scope of this work. Instead, we appeal to the position space representation of the Hofstadter Hamiltonian. It is clear that the spectrum evolves smoothly there because each term in $\mathcal{H}^\phi$ is an analytic function of $\phi$.

8. Embedding Matrices in Flux

Thus far, we have shown that at $\phi = \frac{2\pi p}{q'}$, the Hofstadter Hamiltonian can be diagonalized in a $1 \times q'$ magnetic unit cell, and the magnetic BZ can be taken as $k_1 \in (-\pi, \pi), k_2 \in (0, 2\pi/q')$. This establishes a $2\pi/q'$ periodicity in $k_2$. In this section, we will show that the energy spectrum and eigenstates of the Hofstadter Hamiltonian are also periodic in $k_1$ across the magnetic BZ with period $\phi = \frac{2\pi p}{q'}$, with $p', q'$ coprime. If $\mu$ and $q'$ are coprime, then iterating the $\phi$ periodicity will give a $\frac{2\pi}{q'}$ periodicity in $k_1$, matching the $\frac{2\pi}{q'}$ periodicity along $k_2$. If $\mu$ and $q'$ are not coprime, then iterating the $\phi$ periodicity will only yield a $\frac{2\pi}{q'\gcd(q', \mu)}$ periodicity along $k_1$. In contrast, there will always be a $\frac{2\pi}{q'}$ periodicity along $k_2$ because the magnetic unit cell is $1 \times q'$ at $\phi = \frac{2\pi p}{q'}$, so a $\frac{2\pi}{q'}$ periodicity appears due to the definition of the magnetic BZ. We emphasize that the states at $k$ and $k + \frac{2\pi}{q'} b_1$ are independent states in the Hilbert space although they have the same energy, but states at $k$ and $k + \frac{2\pi}{q'} b_2$ are not independent states due to the definition of the magnetic BZ (see Eq. (A41)). We sketch an example of the magnetic BZ when $\mu = 2$, as is the case for a simple choice of basis for the lattice in Fig. 4 and $\phi = \frac{2\pi x_3}{4} = 3\pi$ in Fig. 7 where there is a $\pi$ periodicity along $k_1 \in (-\pi, \pi)$ and a $\frac{2\pi}{q'} = \pi/2$ periodicity along $k_2 \in (0, \frac{\pi}{q'})$.

In our Landau gauge $A(r) = -\phi b_1 (r \cdot b_2)$, we will find expressions for magnetic embedding matrices $V_i(\phi)$ which obey

$$\mathcal{H}^\phi(k + \phi b_1) = V_i(\phi) \mathcal{H}^\phi(k) V_i^\dagger(\phi)$$  \hspace{1cm} (A43)

and implement the $\phi$ periodicity in the spectrum. This is the same $\phi$ periodicity that was proved in Eq. (4) using the magnetic translation operators. The energy spectrum always has a $\phi$ periodicity along both axes of the magnetic BZ, no matter what magnetic unit cell is chosen to diagonalize the Hamiltonian.

We begin with the expression for $V_2(\phi)$ in our Landau gauge, noting that

$$c_{k_1, k_2 + \phi, \ell, \alpha} = \frac{1}{\sqrt{N/q'}} \sum_{r_1r_2} e^{i(k + b_2 \phi) \cdot (r_1a_1 + q' r_2 a_2 + \ell a_2 + \delta_\alpha)} C_{r_1r_2, \ell, \alpha}$$

$$= \frac{1}{\sqrt{N/q'}} \sum_{r_1r_2} e^{i(k - \phi a_1 + q' r_2 a_2 + \ell a_2 + \delta_\alpha)} e^{i\phi(q' r_2 + \ell + b_2 \frac{2\pi}{q'})} C_{r_1r_2, \ell, \alpha}$$

$$= \frac{1}{\sqrt{N/q'}} \sum_{r_1r_2} e^{i(k - \phi a_1 + q' r_2 a_2 + \ell a_2 + \delta_\alpha)} e^{i\phi(\ell + b_2 \frac{2\pi}{q'})} C_{r_1r_2, \ell, \alpha}$$

$$= \sum_{\ell' \beta} [V_2(\phi)]_{\ell, \alpha, \ell', \beta} c_{k_1, k_2, \ell', \beta}$$  \hspace{1cm} (A44)

where we have defined

$$[V_2(\phi)]_{\ell, \alpha, \ell', \beta} = \delta_{\ell' \ell} e^{-i\phi \delta_\alpha \delta_\beta} e^{i\phi \delta_\beta} b_2 .$$  \hspace{1cm} (A45)

This allows us to deduce the action of $V_2$ on the Hamiltonian:

$$H^\phi = \sum_{k_1, k_2} \sum_{\ell, \alpha, \ell', \beta} c_{k_1, k_2, \ell, \alpha}^\dagger [\mathcal{H}(k_1, k_2)]_{\ell, \alpha, \ell', \beta} c_{k_1, k_2, \ell', \beta}$$

$$= \sum_{k_1, k_2} \sum_{\ell, \alpha, \ell', \beta} c_{k_1, k_2, \ell, \alpha}^\dagger [\mathcal{H}(k_1, k_2 + \phi)]_{\ell, \alpha, \ell', \beta} c_{k_1, k_2, \ell', \beta}$$

$$= \sum_{k_1, k_2} \sum_{\ell, \alpha, \ell', \beta} \sum_{\ell'', \alpha', \beta'} c_{k_1, k_2, \ell, \alpha}^\dagger [V_2^\dagger(\phi)]_{\ell', \alpha', \ell, \alpha} [\mathcal{H}(k_1, k_2)]_{\ell, \alpha, \ell', \beta} c_{k_1, k_2, \ell', \beta}$$  \hspace{1cm} (A46)
Matching terms, we see that Eq. (A43) is satisfied. We note that $V_2(\phi)$ is a diagonal matrix of phases, and so is unitary.

To derive $V_1(\phi)$ in our Landau gauge, we focus without loss of generality on a generic hopping of $H^\phi$ from $r_1a_1 + (q' r_2 + \ell')a_2 + \delta_\alpha$ to $r_1' a_1 + (q' r_2' + \ell')a_2 + \delta_\beta$. Let $(\Delta_1, \Delta_2) = (r_1' - r_1, q' (r_2 - r_2') + \ell' - \ell)$ denote the distance between the unit cells of the orbitals in the hopping, and let $t$ denote the amplitude of the hopping. After Fourier transforming this hopping, we get a term in the Hamiltonian Eq. (A12) given by

$$[\mathcal{H}_t^\phi(k)]_{\ell, \alpha, \ell', \beta} = t e^{i \varphi_{\ell, \alpha, \ell', \beta}} - i k_1 b_1 \cdot \Delta_1 a_1 + \delta_\alpha - \delta_\beta, \quad (A47)$$

and the whole Hamiltonian $\mathcal{H}_t^\phi(k)$ consists of a sum over the hoppings $t$ of $\mathcal{H}_t^\phi(k)$. We recall that $\varphi_{\ell, \alpha, \ell', \beta}$ is the Peierls phase (see Eq. (A30) and the following discussion). Using the expression for $\mathcal{H}_t^\phi(k_1, k_2)$ in Eq. (A47), we see that

$$[\mathcal{H}_t^\phi(k_1 + \phi, k_2)]_{\ell-1, \alpha, \ell'-1, \beta} = [\mathcal{H}_t^\phi(k_1, k_2)]_{\ell, \alpha, \ell', \beta} . \quad (A48)$$

where $\ell$ and $\ell'$ are defined mod $q'$. Now we calculate that

$$\varphi_{\ell-1, \alpha, \ell'-1, \beta} - \phi b_1 \cdot (\Delta_1 a_1 + \delta_\alpha - \delta_\beta) = - \phi \int_{r_1 a_1 + (\ell-1+q' r_2) a_2 + \delta_\alpha} (r \cdot b_2) b_1 \cdot dr - \phi b_1 \cdot (\Delta_1 a_1 + \delta_\alpha - \delta_\beta)$$

$$= - \phi \int_{r_1 a_1 + (\ell-1+q' r_2) a_2 + \delta_\alpha} ((r - a_2) \cdot b_2) b_1 \cdot dr - \phi b_1 \cdot (\Delta_1 a_1 + \delta_\alpha - \delta_\beta)$$

$$= \varphi_{\ell, \alpha, \ell', \beta} + \phi \int_{r_1 a_1 + (\ell+q' r_2) a_2 + \delta_\alpha} b_1 \cdot dr - \phi b_1 \cdot (\Delta_1 a_1 + \delta_\alpha - \delta_\beta)$$

$$= \varphi_{\ell, \alpha, \ell', \beta} + \phi b_1 \cdot (\Delta_1 a_1 + \delta_\alpha - \delta_\beta) - \phi b_1 \cdot (\Delta_1 a_1 + \delta_\alpha - \delta_\beta)$$

where we have used $a_2 \cdot b_2 = 1$. We observe that the cancelation of the $\Delta_1$-dependent terms is due to the structure of our Landau gauge. Comparing Eqs. (A47) and (A48), we see that

$$[\mathcal{H}_t^\phi(k_1 + \phi, k_2)]_{\ell-1, \alpha, \ell'-1, \beta} = [\mathcal{H}_t^\phi(k_1, k_2)]_{\ell, \alpha, \ell', \beta} . \quad (A50)$$

Hence, defining

$$[V_1(\phi)]_{\ell, \alpha, \ell', \beta} = \delta_{\ell, \ell'} \delta_{\alpha, \beta}, \quad (A51)$$

emphasizing again that $\ell$ and $\ell'$ are defined mod $q'$ in the Kronecker delta. We find that $\mathcal{H}_t^\phi(k_1 + \phi, k_2) = V_1(\phi) \mathcal{H}_t^\phi(k_1, k_2) V_1^\dagger(\phi)$. Note that $V_1(\phi)$ is unitary because it is the tensor product of a permutation matrix and the identity. Thus we have proven Eq. (A43) holds for $H^\phi$ when focusing on a single generic hopping. It is simple to extend this result for $H^\phi$ having arbitrary hoppings. We observe that

$$\mathcal{H}_t^\phi(k_1, k_2) = \sum_{\text{hoppings } t} \mathcal{H}_t^\phi(k_1, k_2)$$

$$\mathcal{H}_t^\phi(k_1 + \phi, k_2) = \sum_{\text{hoppings } t} \mathcal{H}_t^\phi(k_1 + \phi, k_2)$$

$$= \sum_{\text{hoppings } t} V_1(\phi) \mathcal{H}_t^\phi(k_1, k_2) V_1^\dagger(\phi) \quad (A52)$$

$$= V_1(\phi) \left( \sum_{\text{hoppings } t} \mathcal{H}_t^\phi(k_1, k_2) \right) V_1^\dagger(\phi)$$

$$= V_1(\phi) \mathcal{H}_t^\phi(k_1, k_2) V_1^\dagger(\phi) .$$

By explicit computation, we obtain the braiding relation of the embedding matrices,

$$V_1(\phi) V_2(\phi) = e^{i\phi} V_2(\phi) V_1(\phi) . \quad (A53)$$

According to Eq. (A43), the embedding matrices $V_1(\phi)$ establish a $\phi$ periodicity along $k_1$ and $k_2$ in the energy spectrum.
We follow the steps of Eq. (A44) and find
\begin{equation}
H^{\phi=0}(k + 2\pi b_i) = V_i H^{\phi=0}(k) V_i^\dagger.
\end{equation}
We extend this embedding matrix to the nonzero flux case to recover the usual 2\pi periodicity in the magnetic BZ by defining its action on the Hofstadter Hamiltonian as the identity on the \ell indices, i.e. \([V_i]_{\alpha,\beta} \rightarrow [V_i]_{\ell,\ell'} = \delta_{\ell,\ell} \delta_{\alpha,\beta} e^{2\pi i \delta_{\alpha,\beta}} \), such that
\begin{equation}
H^{\phi}(k + 2\pi b_i) = V_i H^{\phi}(k) V_i^\dagger.
\end{equation}

It is sometimes useful to combine the 2\pi periodicity given by \(V_i\) and the \(\phi\) periodicity given by \(V_i(\phi)\). For example at \(\phi = \frac{2\pi}{q}\), the spectrum is actually \(\frac{2\pi}{q}\)-periodic, as we see from iterating the \(\phi = \frac{2\pi}{q}\) periodicity twice, and then applying the 2\pi periodicity of \(k_1\) given by \(V_i\). The embedding matrix \(V_i^\dagger V_i(\phi)^2\) establishes this \(\frac{2\pi}{q}\)-periodicity. By combining the \(\phi\) periodicity and the 2\pi periodicity, we will show that there is a \(\frac{2\pi}{q}\) periodicity along \(k_1\) at \(\phi = \frac{2\pi p}{q} = \mu \frac{2\pi q'}{q}\). Note that the periodicity along \(k_1\) depends on \(q\) and is gauge-independent. This \(2\pi/q\) periodicity along \(k_1\) is the same as the periodicity established by the magnetic translation group in Eq. (4).

To find expressions for the embedding matrices that implement the \(\frac{2\pi}{q}\) periodicity, we define \(\zeta, s \in \mathbb{Z}\) by
\begin{equation}
\zeta \phi = \frac{2\pi}{q} + 2\pi s.
\end{equation}

or equivalently \(\zeta \phi = 2\pi/q \mod 2\pi\). To prove the \(\frac{2\pi}{q}\) periodicity along \(k_1\), we first note that
\begin{equation}
H^{\phi}(k + \zeta \phi b_i) = [V_i(\phi)]^\zeta H^{\phi}(k) [V_i^\dagger(\phi)]^\zeta.
\end{equation}

Additionally, we see
\begin{equation}
H^{\phi}(k + \zeta \phi b_i) = \frac{2\pi}{q} b_i + 2\pi s b_i
\end{equation}
\begin{equation}
\left( [V_i]^{\ast} [V_i] \right)^\zeta
\end{equation}
\begin{equation}
\end{equation}

Combining Eqs. (A57) and (A58), we obtain
\begin{equation}
H^{\phi}(k + \frac{2\pi}{q} b_i) = \tilde{V}_1(\phi) H^{\phi}(k) \tilde{V}_1^\dagger(\phi), \quad \tilde{V}_1(\phi) = [V_i^\dagger]^\ast [V_i(\phi)]^\zeta\end{equation}

which shows the spectrum is \(2\pi/q\)-periodic along \(k_1\). We remark that \([V_i, V_i(\phi)] = 0\). The algebra of \(\tilde{V}_1\) and \(\tilde{V}_2\) is readily obtained by repeated application of Eq. (A53) and Eq. (A56). We find
\begin{equation}
\tilde{V}_1(\phi) \tilde{V}_2(\phi) = e^{i e^{2\pi i q} \tilde{V}_2(\phi) \tilde{V}_1(\phi)}.
\end{equation}

We have thus far shown that \(V_i(\phi)\) and \(V_2(\phi)\) give a \(\phi\) periodicity along \(k_1\) and \(k_2\). Also we combined the \(\phi\) and \(2\pi\) periodicity along \(k_1\) to show that \(\tilde{V}_1(\phi)\) gives a minimal \(\frac{2\pi}{q}\) periodicity along \(k_1\) at \(\phi = \frac{2\pi p}{q}\). Recall from App. A5 that \(q'\) is an integer multiple of \(q\), and \(\frac{q}{q'} = \mu\) when \(\mu\) and \(q'\) are coprime. We emphasize that \(k_1\) is periodic in \(\frac{2\pi}{q}\). However, we will now show that because the magnetic BZ is given by \(k_1 \in (-\pi, \pi), k_2 \in (0, 2\pi/q')\), \(k_2\) is periodic in \(\frac{2\pi}{q'}\) which is a finer periodicity, and implies a larger \(\frac{2\pi}{q}\) periodicity along \(k_2\) when iterated. We now construct the embedding matrix \(\tilde{V}_2(\phi)\) that gives the \(\frac{2\pi}{q}\) periodicity along \(k_2\). This periodicity arises because we diagonalized the Hamiltonian in a \(1 \times q'\) magnetic unit cell and is gauge dependent. \(\tilde{V}_2(\phi)\) satisfies
\begin{equation}
H^{\phi}(k + \frac{2\pi}{q'} b_2) = [\tilde{V}_2(\phi)] H^{\phi}(k) [\tilde{V}_2(\phi)]^\dagger.
\end{equation}

We follow the steps of Eq. (A44) and find
\begin{equation}
\begin{aligned}
c_{k_1, k_2 + \frac{2\pi}{q'} b_2, \ell, \alpha} &= \sum_{r_1, r_2} e^{i (k + b_2 \frac{2\pi}{q'}) \cdot (r_1 a_1 + q' r_2 a_2 + \ell a_2 + \delta_\alpha)} c_{r_1, r_2, \ell, \alpha} \\
&= \sum_{r_1, r_2} e^{i (r_1 a_1 + q' r_2 a_2 + \ell a_2 + \delta_\alpha)} e^{i \frac{2\pi}{q'} (q' r_2 + \ell + b_2 \delta_\alpha)} c_{r_1, r_2, \ell, \alpha} \\
&= [\tilde{V}_2(\phi)]_{\ell, \alpha, \ell', \beta} c_{k_1, k_2, \ell', \beta}.
\end{aligned}
\end{equation}
\[ \phi = 3\pi, \mu = 2, p' = 3, q' = 4 \]

![Diagram](image)

**FIG. 7.** We show the magnetic BZ at \( \phi = 2\frac{2\pi \times 3}{4} = 3\pi \) with \( \mu = 2 \) and \( q' = 4 \) not coprime, and \( p' = 3 \). There is a \( \pi \) periodicity along \( k_1 \) implemented by \( \tilde{V}_1(\phi) \), but a \( \pi/2 = 2\pi/q' \) periodicity along \( k_2 \) implemented by \( \tilde{V}_2(\phi) \) because the magnetic BZ is defined as \( k_1 \in (-\pi, \pi), k_2 \in (0, \pi/2) \). The embedding matrices \( \tilde{V}_2(\phi) = [\tilde{V}_2(\phi)]^2 \) or \( \tilde{V}_2(\phi) = [\tilde{V}_2(\phi)]^6 \) implement periodicities that are larger than the domain of \( k_2 \).

with

\[
[\tilde{V}_2(\phi)]_{\ell,\alpha,\ell',\beta} = \delta_{\ell\ell'}e^{i\frac{2\pi}{q'}\ell}e^{i\frac{2\pi}{p'}\delta_{\alpha\beta}}b_2. \tag{A63}
\]

We observe from Eqs. (A63) and (A45) that \( \tilde{V}_2(\phi)^{p'q'} = V_2(\phi) \). The algebra with with \( V_1(\phi) \) can be directly computed and reads

\[
V_1(\phi)\tilde{V}_2(\phi) = e^{i\frac{2\pi}{q'}\tilde{V}_2(\phi)V_1(\phi)}. \tag{A64}
\]

In App. C1 we will need the algebra of \( \tilde{V}_2(\phi) \) with \( \tilde{V}_1(\phi) \) to study the Wilson loop in the magnetic BZ. Using Eq. (A64) and the definition of \( \tilde{V}_1(\phi) \) in Eq. (A59), we arrive at

\[
\tilde{V}_1(\phi)\tilde{V}_2(\phi) = e^{i\frac{2\pi}{q'}\tilde{V}_2(\phi)\tilde{V}_1(\phi)}. \tag{A65}
\]

We depict the magnetic BZ and embedding matrices for \( \phi = 2\frac{2\pi \times 3}{4} = 3\pi \), with \( \mu = 2 \) and \( p = 3, q' = 4 \) in Fig. 7. Note that \( \mu \) and \( q' \) are not coprime, so the periodicities along \( k_1 \) (which is \( \pi \)) and \( k_2 \) (which is \( \pi/2 \)) are not equal.

We now give a brief example illustrating the different embedding matrices. In App. A5 we discussed a model on the square lattice with 1a and 1b atoms (see Fig. 4) where \( \mu = 2 \) for \( a_1 = (1,0), a_2 = (0,1) \). In our Landau gauge defined by \( \mathbf{A}(\mathbf{r}) = -\phi \mathbf{b}_1(\mathbf{r} \cdot \mathbf{b}_2) = \phi(-y,0) \), the Hofstadter Hamiltonian could be formed by taking \( \phi = 2\frac{2\pi p'}{q'} \) for \( p' \) and \( q' \) coprime, and defining the magnetic BZ as \( k_1 \in (-\pi, \pi), k_2 \in (0, 2\pi/q') \). The \( \tilde{V}_1(\phi) \) embedding matrix provides a \( 2\pi/q \) periodicity in the energy spectrum along \( k_1 \) and \( k_2 \), where \( \phi = 2\frac{2\pi p'}{q'} \) and \( p \) and \( q \) coprime. Due to \( \tilde{V}_2(\phi) \), there is always a \( 2\pi/q' \) periodicity along \( k_2 \). In this example, when \( q' \) and \( \mu = 2 \) are not coprime (i.e. \( q' \) is even), we have \( \frac{2\pi}{q'} = \frac{\pi}{2} \), and so \( k_2 \) has twice a fine a periodicity as \( k_1 \). When \( q' \) and \( \mu = 2 \) are coprime, both \( k_1 \) and \( k_2 \) have the same periodicity.

**Appendix B: Bounded Gaps in the Trivial Limit**

In this Appendix, we prove that a Hamiltonian with a large enough on-site, per orbital, potential has a gapped Hofstadter Butterfly spectrum for any flux and hence is adiabatically connected to the atomic limit for all flux (App. B1). Such a property was mentioned in the derivation of the bulk gap closing of an insulator with nonzero Chern number in Sec. of the main text. We exemplify this feature on the checkerboard lattice model in App. B2.

1. Gershgorin circles

We first consider the Hamiltonian at zero field. We add to the lattice model described by the hopping amplitudes \( t_{\alpha\beta}(\mathbf{r} - \mathbf{r}') \) an on-site, per-orbital potential

\[ \mu_\alpha = (2\alpha - N_{orb} - 1)M \tag{B1} \]
where \( \alpha = 1, \ldots, N_{\text{orb}} \) labels the orbitals and \( M \) is the on-site amplitude. Let \( H \) be the matrix representation of the tight-binding hamiltonian in real space including both \( \mu_\alpha \) and the hopping amplitudes. \( H \) is a \((N_{\text{orb}}N) \times (N_{\text{orb}}N)\) hermitian matrix where \( N \) is the number of unit cells. We want to focus on the eigenvalues of \( H \). Thanks to the translation invariance, we can define \( N_{\text{orb}} \) Gershgorin circles \( D_\alpha \) of center \( \mu_\alpha \) and radius \( R_\alpha \) with

\[
R_\alpha = \sum_{\beta \neq \alpha} \sum_r |t_{\alpha\beta}(r)|. \tag{B2}
\]

We assume that these series appearing in Eq. \[ B2 \] do converge, which is true for any system with only finite range hopping terms or exponentially decaying hoppings \( |t_{\alpha\beta}(r)| \sim \exp(-\kappa |r|), \kappa > 0 \), as may arise in the case of flat Chern bands \[ 43, 44 \]. From there we define \( R_{\text{max}} = \max \{ R_\alpha; \alpha = 1, \ldots, N_{\text{orb}} \} \). The Gershgorin circle theorem states that any eigenvalue of \( H \) lies within at least one of the Gershgorin circles, and a union of \( m \) circles disjoint from all other circles must contain exactly \( m \) eigenvalues of \( H \). For \( |M| \) large, i.e., in the atomic limit, we have exactly \( N \) eigenvalues lying in each \( D_\alpha \) circle, forming \( N_{\text{orb}} \) separated trivial bands. As long as \( |M| > R_{\text{max}} \), we are guaranteed that all the \( D_\alpha \) circles are disjoint and thus all bands are separated by a gap from above and below, as we sketch in Fig. 8a.

Turning on the magnetic field, the hopping terms acquire a phase \( t_{\alpha\beta}(r-r') \rightarrow t_{\alpha\beta}(r-r') \exp \left[ i \int_{R+\delta_{x}}^{R+\delta_{y}} \mathbf{A} \cdot \mathbf{dr} \right] \) from the Peierls substitution as discussed in App. \[ A1 \]. Note that \( \mu_\alpha \) and \( R_\alpha \) are unchanged under this substitution and so are the \( D_\alpha \) circles. This implies that for \( |M| > R_{\text{max}} \) and irrespective of the magnetic field, the Gershgorin circles remain disjoint and each band is gapped. As a consequence, if we start with \( N_{\text{occ}} \) occupied bands at \( \phi = 0 \), these bands will stay gapped for any \( \phi \neq 0 \) if \( |M| > R_{\text{max}} \). This is valid subject to the convergence of the sum in Eq. \[ B2 \]. This is not in contradiction to Sec. where we proved that a model with nonzero Chern number necessarily has a gap closing: for large enough \( |M| \), i.e. \( |M| > R_{\text{max}} \), the model cannot host nontrivial bands because it is adiabatically connected to an atomic limit. When \( M < R_{\text{max}} \), a gap closing is not forbidden in the Hofstadter spectrum.

2. Hofstadter Hamiltonian on the Checkerboard Lattice

We consider a checkerboard lattice with \( s \) orbitals at the 1a position \( (0,0) \) and 1d position \( (1/2, 1/2) \) positions \[ 45, 46 \]. In the basis \( c_R^\dagger = (c_{R,1a}^\dagger, c_{R,1d}^\dagger) \), the Hamiltonian is given by

\[
H^{\phi=0} = \sum_{\mathbf{R}} M_{\mathbf{R}} c_{\mathbf{R}}^{\dagger} \sigma_z c_{\mathbf{R}} + t \sum_{\mathbf{R}} \sum_{j} c_{\mathbf{R}+\mathbf{d}_j}^{\dagger} (\sigma_1 \cos \theta + (-1)^j \sigma_2 \sin \theta) c_{\mathbf{R}} + t' \sum_{\mathbf{R}} c_{\mathbf{R}+\mathbf{d}_1}^{\dagger} \sigma_z c_{\mathbf{R}} - c_{\mathbf{R}+\mathbf{d}_3}^{\dagger} \sigma_z c_{\mathbf{R}} + h.c. \tag{B3}
\]

where \( \mathbf{d}_j \) are defined by \( \mathbf{d}_0 = 0, \mathbf{d}_1 = -\hat{x}, \mathbf{d}_2 = -\hat{x} - \hat{y}, \mathbf{d}_3 = -\hat{y} \). The hoppings \( t (t') \) represent nearest (next-nearest) neighbor hoppings as shown in Fig. 8b and Fig. 8c. Note that the parameter \( M \) matches the definition of the on-site...
potential \( \mu_a \) Eq. [B1] We use the parameters \( t = 1, t' = 1/2, \theta = \pi/4 \). At \( \phi = 0 \), the model is topological with \( C = 1 \) for \( |M| < 2 \), and for \( |M| > 2 \), the model is in a trivial atomic limit.

We introduce magnetic flux through the lattice in our Landau gauge \( A = -\phi(y, 0) \) and take each Peierls integral along the straight-line paths between the endpoints. This is the conventional choice for \( s \) orbitals. Our choice for the Peierls paths allows minimal loops that enclose \( 1/4 \) along the straight-line paths between the endpoints. This is the conventional choice for the Wannier centers of the magnetic unit cell, due to the magnetic translation group (App. C 1). In App. C 2, we provide analysis can produce tighter bounds.

where the Peierls phases are given by

\[
H^{\phi} = \sum_{\mathbf{R}} M \mathbf{c}_{\mathbf{R}+\mathbf{d}} \mathbf{c}_{\mathbf{R}} + \sum_{\mathbf{R}} \sum_j c_{\mathbf{R}+\mathbf{d}_j} \left[ \begin{pmatrix} 0 & t_j(\phi) \cos \theta + (-1)^j \sin \theta \\ 0 & -i t_j(\phi)^* \end{pmatrix} \right] c_{\mathbf{R}} + \sum_{\mathbf{R}} c_{\mathbf{R}+\mathbf{d}} \left[ \begin{pmatrix} t_{1,a}^{R}(\phi) & 0 \\ 0 & -t_{1,d}^{R}(\phi) \end{pmatrix} c_{\mathbf{R}} - t' c_{\mathbf{R}+\gamma} \sigma \mathbf{c}_{\mathbf{R}} + h.c. \right.
\]

(B4)

where the Peierls phases are given by

\[
t_j(\phi) = t e^{i f_{\mathbf{R}+\mathbf{d}_j} A \cdot \mathbf{r}} = \{ t e^{-i \mathbf{d}_j \cdot \mathbf{R} + \frac{1}{2} \mathbf{R} \cdot \mathbf{\delta}}, t e^{i \mathbf{d}_j \cdot \mathbf{R} + \frac{1}{2} \mathbf{R} \cdot \mathbf{\delta}}, t e^{i \mathbf{d}_j \cdot \mathbf{R} - \frac{1}{2} \mathbf{R} \cdot \mathbf{\delta}}, t e^{-i \mathbf{d}_j \cdot \mathbf{R} - \frac{1}{2} \mathbf{R} \cdot \mathbf{\delta}} \}.
\]

(B5)

Using Eq. (A28), we compute \( \mu = \text{gcd} \{ b_1 \cdot (\mathbf{\delta} - \mathbf{d}_a) \} = \text{gcd} \{ 1, 1/2 \} = 2 \) because there are orbitals at \( 1a = (0, 0) \) and \( 1a = (1/2, 1/2) \) connected by a hopping. Indeed, from the Peierls phases themselves, we see that setting \( \phi = \frac{2 \pi q'}{q} \) gives a \( 1 \times q' \) unit cell, meaning the phases Eq. (B5) are invariant under \( y \rightarrow y + q' \).

We define the Hermitian matrices

\[
\Sigma_j(k_x, k_y) = \begin{pmatrix}
0 & t_j(\phi) e^{ik \cdot (\mathbf{d} + \mathbf{d}_j)} e^{i(k_x + \mathbf{d}_j)} \\
0 & 0
\end{pmatrix}
\]

(B6)

where the location of the 1d Wyckoff position is \( \mathbf{\delta} = (1/2, 1/2) \). We Fourier transform over the magnetic unit cell at \( \phi = 2 \frac{2 \pi q'}{q} \) to find

\[
\begin{align*}
H_{y, y'}^{\phi} &= \delta_{y, y'} h_y + \delta_{y, y' + i} T_y(y') + \delta_{y + 1, y'} T^y_y \\
&= M \sigma_z + \sum_{k_x, k_y} \left[ \cos(k_x + \phi y) 0 \\
&- \cos(k_x + \phi y/2) \right] - 2 t' \left[ \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} e^{ik \cdot (\mathbf{d} + \mathbf{d}_3)} e^{i\theta t_5(\phi)^* e^{ik \cdot (\mathbf{d} + \mathbf{d}_3)}} - t' \sigma_z e^{-ik_y} \right]
\end{align*}
\]

(B7)

where \( y = 0, \ldots, q' - 1 \) at \( \phi = 2 \frac{2 \pi q'}{q} \).

We numerically diagonalize this Hofstadter Hamiltonian Eq. (B7) to compute the Hofstadter Butterfly at \( M = 2.4 \) in Fig. 9. The two Gershgorin circles for the checkerboard lattice model are defined by the two centers \( \mu_{1a} = |M| \) and \( \mu_{1d} = -|M| \), and the Gershgorin radius \( R_{\text{max}} = R_{1a} = R_{1d} = 4 (|t| + |t'|) \) (each site being connected to four nearest neighbors and four next nearest neighbors). For the parameters used in Fig. 9 we get \( R_{\text{max}} = 6 \). For any \( |M| > 4 \), we are guaranteed that the system at half filling will have a gap irrespective of \( \phi \). Note that this value is only an upper bound of the minimal \( |M| \) value where this gap can appear. As already mentioned previously, the transition from a \( C = 1 \) topological band to a trivial band occurs at \( |M| = 2 \), and for \( M > 2 \) the Hofstadter Butterfly is gapped everywhere. We show an example of the Hofstadter Butterfly in this phase in Fig. 9. It is hence expected that further analysis can produce tighter bounds.

Appendix C: Wilson Loops

In this Appendix, we define the Wilson loop at nonzero flux and determine the constraints on its eigenvalues, the Wannier centers of the magnetic unit cell, due to the magnetic translation group (App. C 1). In App. C 2, we provide
an alternative proof of the major claim in Sec. , that $C_{\phi}^{\phi=2\pi q} \in q\mathbb{Z}$, which leads to a proof of gap closing in the bulk of the Hofstadter Butterfly when the $\phi = 0$ model has a nonzero Chern number. We also discuss in depth the behavior of the occupied bands as the flux is pumped. In App. [C3] we show that a Mirror Chern number also enforces a gap closing. We provide an alternative proof of the gap closing for a nonzero Chern number using only inversion eigenvalues (App. [C4]).

1. Definition of the Wilson Loop at Nonzero Flux

The Wilson loop at $\phi = 0$ is calculated from the eigenvectors of $H^0(k)$. Denote the $j$th eigenvector as $|u_j(k)\rangle$, which is a vector with $N_{\text{orb}}$ components corresponding to the $j$th eigenvalue $\epsilon_j(k)$. (Note that this is a slight abuse of the ket notation, which usually specifies a state in the Hilbert space, as opposed to merely a vector in $\mathbb{R}^N$.) We denote the $i$th element of the $j$th (ordered by energy) eigenvector by $|u_{ij}(k)\rangle$, $i = 1, \ldots, N_{\text{orb}}$. When the bulk spectrum is gapped, we may consider only the $N_{\text{occ}} < N_{\text{orb}}$ occupied bands which determine the topology of the Hamiltonian at a given filling $\nu = N_{\text{occ}}/N_{\text{orb}}$. For brevity, we write $[U_{12}] = |u_{ij}(k)\rangle_i$ as the matrix of occupied eigenvectors. (Here we assume the bulk spectrum is gapped so the occupied spectrum is well-defined.) Then the Wilson loop is defined by

$$W_{\phi=0}(k_1) = U_{(k_1,2\pi)}^\dagger \prod_{k_2}^{2\pi \rightarrow 0} P_{(k_1,k_2)} U_{(k_1,0)}, \quad P_{(k_1,k_2)} = U_{(k_1,k_2)} U_{(k_1,k_2)}^\dagger$$

(C1)

where the ordered product is understood to be discretized: $\prod_{k_2}^{2\pi \rightarrow 0} P_{(k_1,k_2)} \equiv \lim_{\epsilon \rightarrow 0} P_{(k_1,2\pi)} P_{(k_1,2\pi-\epsilon)} \cdots P_{(k_1,0)}$. It is convenient to fix the $U(1)$ gauge symmetry of the eigenvalues by requiring $U_{(k_1,2\pi)} = V_2 U_{(k_1,0)}$.

When we add flux to the model in our Landau gauge, the magnetic BZ can be chosen to be $k_1 \in (-\pi, \pi), k_2 \in (0, \frac{2\pi}{q})$ as discussed in App. [A7]. To define the Wilson loop along the $k_2$ direction of the BZ at $\phi = \frac{2\pi q}{q}$, we assume there is a set of $N_{\text{occ}}^\phi$ occupied bands which are gapped from the higher energy bands whose eigenvectors form the matrix $[U_{12}^\phi] = |u_{ij}^\phi(k)\rangle_i$. Then we may calculate the Wilson loop according to

$$W_{(k_1,\frac{2\pi}{q})\rightarrow(k_1,0)} \equiv W_{\phi=\frac{2\pi q}{q}}(k_1) = [U_{(k_1,\frac{2\pi}{q})}^\phi]^\dagger \prod_{k_2}^{\frac{2\pi}{q} \rightarrow 0} P_{(k_1,k_2)}^{\phi} U_{(k_1,0)}^{\phi} .$$

(C2)

We have chosen to take the Wilson loop along the $k_2$ direction so the Wilson loop eigenvalues correspond to positions along the extended $a_2$ direction of the magnetic unit cell [47]. We will usually be interested in the Wilson loop at the
fixed filling $\nu = N_{\text{occ}}/N_{\text{orb}}$ of the zero-field Hamiltonian. In this case at filling $\nu$, $N_{\text{occ}} \equiv \frac{2\pi}{q'} = q' N_{\text{occ}}$ because there are $q' N_{\text{orb}}$ bands in $H^\phi$ due to the magnetic unit cell being $1 \times q'$. (Of course, it is possible for gaps to exist at other fillings in the Hofstadter Hamiltonian at a given flux.) As in the zero-field case, it is convenient to fix the gauge by requiring

$$U^\phi_{(k_1, \frac{2\pi}{q})} = \mathcal{V}_2(\phi) U^\phi_{(k_1, 0)}$$  \hspace{1cm} (C3)

with the embedding matrix $\mathcal{V}_2(\phi)$ providing the $2\pi/q'$ periodicity in $k_2$ (see Eq. (A62)).

We study the effect of the magnetic translation group on the Wilson loop following the presentation of Ref. 35 (App. VII D) which develops constraints on the Wilson loop for tight-binding models with the general symmetry

$$g_B \mathcal{H}(k) g_B^\dagger = \mathcal{H}(D_B k)$$  \hspace{1cm} (C4)

where $D_g$ is an operator acting on the momentum vector. In the Hofstadter Hamiltonian, the magnetic translation group requires $\tilde{V}_1(\phi) \mathcal{H}^\phi(k) \tilde{V}_1^\dagger(\phi) = \mathcal{H}^\phi(k + \frac{2\pi}{q} b_1)$ where $\phi = \frac{2\pi p}{q}, p, q \text{ coprime}$ (see Eq. (A59)). This allows us to form a sewing matrix between the occupied bands at $k$ and $k + \frac{2\pi}{q} b_1$ defined by

$$B^{ij}_k = \langle u^\phi_i(k + \frac{2\pi}{q} b_1) | \tilde{V}_1(\phi) | u^\phi_j(k) \rangle, \quad i, j = 1, \ldots, q' N_{\text{occ}}.$$  \hspace{1cm} (C5)

This matrix is unitary as long as there is a gap above the occupied bands [47] (if there is a gap at $k_1$, there is also a gap at $k_1 + \frac{2\pi}{q}$). Ref. 35 demonstrates that the sewing matrix also obeys

$$|u^\phi_j(k)\rangle = \sum_i \tilde{V}_1(\phi) | u^\phi_i(k + \frac{2\pi}{q} b_1) \rangle B^{ij}_k.$$  \hspace{1cm} (C6)

This prepares us to calculate a small segment of a Wilson line. We find

$$|W^\phi_{(k') - k}\rangle = \langle u^\phi_i(k_1) | u^\phi_j(k_1) \rangle 
= \sum_{rs} B^{ij}_k | \tilde{V}_1(\phi) | u^\phi_i(k) \rangle B^{ij}_k \tilde{V}_1^\dagger(\phi) | u^\phi_j(k) \rangle |W^\phi_{(k') - k}\rangle$$

$$= \sum_{rs} B^{ij}_k | \tilde{V}_1(\phi) | u^\phi_i(k) \rangle B^{ij}_k \tilde{V}_1^\dagger(\phi) | u^\phi_j(k) \rangle.$$  \hspace{1cm} (C7)

We are interested in the Wilson loops $W^\phi(k_1) = W^\phi_{(k_1, \frac{2\pi}{q})}$. Piecing together the single Wilson line transformations, we find

$$B_{(k_1, \frac{2\pi}{q})} W^\phi(k_1) B_{(k_1, 0)}^\dagger = W^\phi(k_1 + \frac{2\pi}{q}).$$  \hspace{1cm} (C8)

Now we must relate $B_{(k_1, \frac{2\pi}{q})}$ to $B_{(k_1, 0)}$ to establish a unitary relation between the Wilson loops at $k_1$ and $k_1 + \frac{2\pi}{q}$. By Eq. (A62), $|u^\phi_j(k_1, \frac{2\pi}{q})\rangle = V_2(\phi) | u^\phi_j(k_1, 0) \rangle$, so returning to Eq. (C5), we obtain

$$B^{ij}_k = \langle u^\phi_i(k_1 + \frac{2\pi}{q} b_1) | \tilde{V}_1(\phi) | u^\phi_j(k_1) \rangle 
= \langle u^\phi_i(k_1 + \frac{2\pi}{q} b_1) | V_2(\phi) \tilde{V}_1(\phi) | u^\phi_j(k_1) \rangle.$$  \hspace{1cm} (C9)

We simplify the product $\tilde{V}_2(\phi) \tilde{V}_1(\phi)$ using the algebra in Eq. (A65). We find

$$B^{ij}_{(k_1, \frac{2\pi}{q})} = \langle u_i(k_1 + \frac{2\pi}{q} b_1, 0) | \tilde{V}_2(\phi) e^{i\frac{2\pi}{q} \phi} \tilde{V}_1(\phi) | u_j(k_1, 0) \rangle$$

$$= \left[ \frac{2\pi}{q}, \phi \right] B^{ij}_{(k_1, 0)}.$$  \hspace{1cm} (C10)

relating the sewing matrix $B$ at $k_2 = 0$ and $k_2 = 2\pi/q'$. We remind the reader that $\phi \in \mathbb{Z}$ satisfies $\phi \phi = 2\pi/q \mod 2\pi$. Plugging in this result to Eq. (C8), we establish

$$W^\phi(k_1 + \frac{2\pi}{q}) = e^{i\frac{2\pi}{q} \phi} B_{(k_1, 0)}^\dagger W^\phi(k_1) B_{(k_1, 0)}.$$  \hspace{1cm} (C11)
and hence the eigenvalues $e^{i\vartheta_j(k_1)}$ of the Wilson loop, also called the Wannier centers [47], must satisfy

$$\{\vartheta_j(k_1 + \frac{2\pi}{q})\} = \{\vartheta_j(k_1) + \frac{2\pi}{q}\}.$$  

(C12)

This feature of Wilson spectrum can be used to prove topological properties of the Hamiltonian. Below, we show how these results allow an alternative proof of gap closing in a Chern insulator.

2. Wilson Loop Proof of Gap Closing in a Chern Insulator

The winding of the determinant of the Wilson loop is equal to the Chern number, and we may leverage this fact to constrain $C^{\phi}$ at the filling of $\phi = 0$, $\nu = N_{\text{occ}}/N_{\text{orb}}$, with the results of App. C1. Let us again define $q$ as the denominator of $\phi$, i.e. $\phi = \mu \frac{2\pi}{q'} = \frac{2\pi}{q}$. Then assuming a gap exists so that the Wilson loop is well-defined, we establish that

$$\det \left[ W^{\phi}(k_1 + \frac{2\pi}{q}) \right] = \prod_{j=1}^{q'N_{\text{occ}}} e^{i\vartheta_j(k_1 + \frac{2\pi}{q})}$$

$$= \exp \left( i \sum_{j=1}^{q'N_{\text{occ}}} \left( \vartheta_j(k_1) + \frac{2\pi}{q'} \right) \right)$$

$$= \exp \left( i \sum_{j=1}^{q'N_{\text{occ}}} \vartheta_j(k_1) + 2\pi i \zeta N_{\text{occ}} \right)$$

(C13)

$$= \prod_{j=1}^{q'N_{\text{occ}}} e^{i\vartheta_j(k_1)}$$

$$= \det[W^{\phi}(k_1)]$$

using Eq. (C12). We see that the determinant is periodic in $k_1$ with period $\frac{2\pi}{q}$ and consequently must wind a multiple of $q$ times across the magnetic BZ. This proves $C^{\phi = \frac{2\pi}{q}} \in q\mathbb{Z}$ at the filling $\nu = N_{\text{occ}}/N_{\text{orb}}$. If we were to consider another filling where $H^{\phi}$ is gapped, we see from the above calculation that the determinant would not necessarily be $\frac{2\pi}{q}$ periodic, and the Chern number is not required to be quantized in multiples of $q$.

We now discuss in more detail what it means for $H^{\phi = 0}$ to be an insulator with a gap at filling $\nu$, and yet have a gap closing at $\phi \to 0$ enforced by a nonzero Chern number at filling $\nu$. This apparent discrepancy is due to the discontinuity in the energy spectrum at a fixed filling of $H^{\phi}$. While the entire spectrum evolves continuously in $\phi$, there is no guarantee that the spectrum at a given filling is continuous in $\phi$. This is because the filling is determined by the number of bands, and as we have seen in App. C7, the number of bands of $H^{\phi = \mu \frac{2\pi}{q'}}$ depends on $q'$ and thus is discontinuous everywhere.

To illustrate this, we show examples of Hofstadter Butterflies in Fig. [10] calculated from the Hamiltonian $H_{ch}$ (Eq. [B3]). The phases of $H_{ch}^{\phi = 0}$ are controlled by a single parameter $M$. When $|M| < 2$, $H_{ch}^{\phi = 0}$ has a Chern number $C^{\phi = 0} = 1$ at half filling, and when $|M| > 2$, the Hamiltonian is trivial. In addition to the bulk spectrum, we color the maximum (minimum) of the valence (conduction) bands red in order to show that a branch of the conduction bands connects to the valence bands as $\phi$ approaches zero. Thus, the conduction spectrum is discontinuous at $\phi = 0$, although the valence spectrum is continuous. A gapped Hamiltonian $H^{\phi_1}$ with nonzero Chern number at filling $\nu$ cannot be adiabatically connected to another gapped Hamiltonian $H^{\phi_2}$ at filling $\nu$ in the Hofstadter Butterfly as we argued in Sec. . We note that $C^{\phi = \frac{2\pi}{M}} = 0$ is the only number satisfying $C^{\phi} \in q\mathbb{Z}$ for all $\phi$, and hence a gap which exists at filling $\nu$ for a range of $\phi$ can only have $C^{\phi} = 0$. This is illustrated in Fig. [10]. It appears there that there are continuously connected gaps with $C^{\phi} = 1$. However, these gaps are not at the same filling, and hence can be connected without a gap closing. For instance in Fig. [10], the $C = 1$ gap occurs at filling $5/8$ at $\phi = \pi/2$ and filling $3/4$ at $\phi = \pi$, which are in accordance with the Streda formula $\nu = C^{\phi} + \nu_0$ where $\nu_0 = 1/2$ is the filling of the gap at $\phi = 0$. 


FIG. 10. We show the Hofstadter Butterflies for $H_{ch}$ (Eq. (B3)) for (a) the topological phase, $M = 0$, (b) the topological phase, $M = 0.5$, (c) the topological phase, $M = 1.6$, (d) the trivial phase, $M = 2.4$. We indicate the highest occupied state at half filling and the lowest unoccupied state in red, so the half filling gap occurs between the red lines. In (a), (b), (c), we see that the occupied spectrum at half filling does connect smoothly to the occupied spectrum at $\phi = 0$, but the unoccupied spectrum is discontinuous at $\phi = 0$. In particular, there are conduction bands (those above filling $\nu$) that connect to the valence bands (those at or below filling $\nu$) as $\phi$ approaches 0 despite the zero-field Hamiltonian being a gapped insulator at half filling. We have proven that this is required by the nonzero Chern number of the zero-field Hamiltonian. In (a) where $M = 0$, we see an extreme case where the half-filling gap closes, as it must, at $\phi$ but remains extremely small up until $\phi \sim \frac{3\pi}{4}$, (b) The Hofstadter Butterfly is visibly gapped at half-filling for $0 < \phi < \pi$, and the gap closing at $\phi = 0^+$ is clearer. This is even more exaggerated in (c), closer to the $\phi = 0$ phase transition which happens at $M = 2$. Between (c) and (d), the $\phi = 0$ gap closes, and $H^0$ undergoes a transition from a topological insulator to a trivial insulator. In the Hofstadter Butterfly, this transition manifests itself as the conduction branch detaching from the valence branch at $\phi = 0^+$ at the $M = 2$ phase transition and reconnecting with the conduction branch. In the trivial phase, the half filling gap remains open at all $\phi$.

3. Discussion of Gap Closing due to a Nonzero Mirror Chern Number

We now consider the generalization of this theorem to deduce a gap closing in the bulk spectrum of the Hofstadter Butterfly with a nonzero mirror Chern number at $\phi = 0$. However, unlike the case of a true Chern number, a mirror Chern number does not cause the gap to close immediately at $\phi = 0$, as we see in Fig. 1b of the Main Text.

The proof for the bulk gap closing at finite $\phi$ in a model with nonzero mirror Chern number reduces to the Chern number case because the Hamiltonian may be block-diagonalized using the mirror eigenvalues $\pm i$. Additionally, the Hofstadter Hamiltonian may still be block diagonalized by the mirror symmetry $M_z$. Being the product of inversion and a two-fold rotation, $M_z$ is not broken by flux. We assume the total Chern number is zero, or else there would be a gap closing at $\phi = 0^+$. Then the mirror Chern number is defined by

$$C_{M_z} = \frac{C_{m=i} - C_{m=-i}}{2}$$

where $C_{m=\pm i}$ is the Chern number calculated over the occupied bands with mirror eigenvalue $m = \pm i$. The total Chern number is $C = C_{m=i} + C_{m=-i}$ which we assume to be zero (otherwise, we would have a gap closing as $\phi \to 0$),
I assumed odd, there must be a gap closing between $\phi$ bands in the doubled magnetic unit cell at $\nu = 0$ where we have used that the magnetic translation operators satisfy which obey $\mathbf{k} = -\mathbf{k}$. Recalling that $T_2(\phi) |\mathbf{k}\rangle$ has momentum $\mathbf{k} = -\mathbf{b}_1 = \mathbf{k} - \pi \mathbf{b}_1$, we see that if there are $n_1$ negative inversion eigenvalues at the points $(0, 0)$, then there are also $n_1$ negative inversion eigenvalues at $(\pi, 0)$. Similarly, if there are $n_2$ negative inversion eigenvalues at $(0, \frac{\pi}{2})$, then there are $n_2$ positive ones at $(\pi, \frac{\pi}{2})$. Since there are $2N_{\text{occ}}$ bands in the doubled magnetic unit cell at $\phi = \pi$, we find the total number of negative inversion eigenvalues to be $2n_1 + n_2 + (2N_{\text{occ}} - n_2)$ which is even, so the Chern number must be even (zero included) [48]. Because the $C_{\phi=0}$ is assumed odd, there must be a gap closing between $\phi = 0$ and $\phi = \pi$. 

so a nonzero value of $C_{\phi=0}$ means $C_{m=\pm 1}$ must be nonzero. Thus both mirror eigenvalue blocks have opposite and nonzero Chern numbers. Considering each block individually at their own fillings, we use the standard Chern number result of Sec. to show that a band in each must traverse their individual gaps. Considering the full model, the intersection of the Landau levels of different mirror eigenvalues closes the bulk gap at the $\phi = 0$ filling of the whole model.

4. Alternative Proof of Gap Closing Using Inversion Eigenvalues

We proved in Sec. of the Main Text and independently in App. C2 that a Hamiltonian with a nonzero Chern number had a gap closing at the Fermi level. Here, we show that a weaker version of this statement may be proven with knowledge of only inversion (or $C_{2z}$) eigenvalues. We prove now that an insulator with inversion symmetry and odd Chern number must also have a gap closing.

We will calculate the inversion eigenvalues of $\mathcal{H}(\phi)(\mathbf{k})$ at $\phi = 0$ and $\phi = \pi$. We are able to do so because inversion is not broken by a magnetic field, i.e.

$$\mathcal{I} \mathcal{H}(\phi)(\mathbf{k}) \mathcal{I} = \mathcal{H}(\phi)(-\mathbf{k}), \quad \mathcal{I}^2 = 1,$$

By assumption, the Chern number $C_{\phi=0}$ (at filling $\nu$) at $\phi = 0$ is odd, and can be diagnosed by an odd number of $-1$ inversion eigenvalues [48]. Hence to show a gap closing, we need only show that the Chern number at $\phi = \pi$ is even (at the same filling $\nu$), since a gap closing must occur between phases with differing Chern number under adiabatic evolution.

In the magnetic BZ at $\phi = \pi$, we consider the inversion invariant points $\mathbf{k}^* = (k_1^*, k_2^*) = (0, 0), (0, \frac{\pi}{2}), (\pi, 0), (\pi, \frac{\pi}{2})$ which obey $k_1^* = -k_1$ mod $2\pi$ and $k_2^* = -k_2$ mod $\pi$. Now we study the eigenstates of $\mathcal{H}(\phi=\pi)$ at these points. If $\mathcal{I} |\mathbf{k}\rangle = \xi |\mathbf{k}\rangle$, then

$$\mathcal{I} T_2(\pi) |\mathbf{k}\rangle = \xi T_2(\pi) |\mathbf{k}\rangle = \xi T_2(\pi) T_2^\dagger(\pi) |\mathbf{k}\rangle = \xi e^{-2ik_2} T_2(\pi) |\mathbf{k}\rangle$$

where we have used that the magnetic translation operators satisfy $\mathcal{I} T_2(\phi) \mathcal{I} = T_2(\phi)^\dagger$ which follows directly from Eq. [3]. Recalling that $T_2(\phi) |\mathbf{k}\rangle$ has momentum $\mathbf{k} = -\phi \mathbf{b}_1 = \mathbf{k} - \pi \mathbf{b}_1$, we see that if there are $n_1$ negative inversion eigenvalues at the points $(0, 0)$, then there are also $n_1$ negative inversion eigenvalues at $(\pi, 0)$. Similarly, if there are $n_2$ negative inversion eigenvalues at $(0, \frac{\pi}{2})$, then there are $n_2$ positive ones at $(\pi, \frac{\pi}{2})$. Since there are $2N_{\text{occ}}$ bands in the doubled magnetic unit cell at $\phi = \pi$, we find the total number of negative inversion eigenvalues to be $2n_1 + n_2 + (2N_{\text{occ}} - n_2)$ which is even, so the Chern number must be even (zero included) [48]. Because the $C_{\phi=0}$ is assumed odd, there must be a gap closing between $\phi = 0$ and $\phi = \pi$. 

![Block Diagonalized Mirror Chern Insulator](image_url)
Appendix D: Hofstadter Topology Protected by Time Reversal symmetry

In this Appendix, we study the Hofstadter 3D TI phase in generality. First we determine the properties of $UT$, the effective time-reversal symmetry at $\phi = \Phi/2$ (App. D1). We then give two proofs showing that the $\mathbb{Z}_2$ index protected by $UT$ at $\phi = \Phi/2$ is trivial: one in the magnetic BZ (App. D2) and the other using the Wilson loop (App. D3). These proofs are facilitated by a gauge-invariant formalism, introduced in App. D2b, which makes use of the magnetic translation group to construct the Hofstadter Hamiltonian. From this construction, we also find that $UT$ symmetry at $\phi = \Phi/2$ yields a projective representation of the magnetic space group.

1. Properties of $UT$

First, we discuss time-reversal symmetry (TRS) for the Hofstadter Hamiltonian with a $\phi \to \phi + \Phi$ periodicity in the flux. If the $\phi = 0$ model is $\mathcal{T}$-symmetric then the model at $\phi = \Phi/2$ is $UT$-symmetric. This is because

$$ UTH^{\Phi/2}(UT)\dagger = UH^{-\Phi/2}U\dagger = H^{\Phi/2}, \tag{D1} $$

where $U$ is given by Eq. (A5). We now define the anti-unitary operator $\mathcal{T}$ in position space as

$$ \mathcal{T}^{-1}c_{R,\alpha} = \sum_{\beta'} D_{\alpha\beta}(\mathcal{T})c_{R,\beta} \tag{D2} $$

where the unitary matrix $D_{\alpha\beta}(\mathcal{T})$ is only nonzero when $\delta_{\alpha} = \delta_{\beta}$ (and $\alpha$ and $\beta$ are spin-flipped Kramers’ pairs), i.e. $\mathcal{T}$ is local, onsite. $DD^\dagger = \pm 1$ for spinful/spin-less electrons ($T^2 = \pm 1$). The action of $\mathcal{T}$ flips the flux, taking $\phi \to -\phi$ and hence

$$ \mathcal{T}U\mathcal{T}^{-1} = U\dagger \tag{D3} $$

as may be verified using the position space representations of the operators. From here we conclude $(UT)^2 = UUTUT = UU^\dagger T^2 = T^2$. This result holds for $\Phi = 2\pi n$, $n$ even or odd. Because we study insulators with a nontrivial Kane-Mele invariant, we have $T^2 = -1$. We recall that $UH^{\phi}U\dagger = H^{\phi+\Phi}$ and thus $UT$ also protects a topological classification at $H^{\phi=\Phi/2}$ as per Eq. [6].

2. Gauge-Invariant Proof of the 3D TI phase

In the prior sections, we have worked explicitly in the Landau gauge which enables us do explicit, numerical computations such as computing the energy spectrum or the Wilson loop. In this section, we will prove the triviality of the Kane-Mele $\mathbb{Z}_2$ index $\delta^{\Phi=\Phi/2}$, and do not need to perform explicit computations. Hence we can avoid the cumbersome degeneracies caused by the extended $1 \times q$ magnetic unit cell (see App. [A] by introducing a new formalism which makes use of the magnetic translation operators to study the Hofstadter Hamiltonian in the $1 \times q$ without specifying a gauge. First in App. D2a we will construct the Hofstadter Hamiltonian in this magnetic unit cell in a gauge-invariant manner to facilitate a simple proof that $\delta^{\Phi=\Phi/2} = +1$, with the details of the calculations left to App. D2b.

a. Proof of the Trivial Kane-Mele Index due to Gap Closings at the Phase Transition

Recall from Sec. that we may choose a simultaneous eigenbasis of $T_1(\phi), T_2(\phi)$ where $\phi = \frac{2\pi p}{q}$ for $p, q$ coprime. At $\phi = \Phi/2 = \pi n$ for odd $n$, this means $q = 2$. We study the single-particle states $|\alpha, \ell, k_1, k_2\rangle$ with $\alpha = 1, \ldots, N_{\text{orb}}, \ell = 0, 1$ which are eigenstates of $T_1(\Phi/2)$ and $T_2(\Phi/2)$. Going forward, we write $T_1(\Phi/2) = T_1$ for brevity unless otherwise specified. These states satisfy

$$ T_1 |k_1, k_2, \ell, \alpha\rangle = e^{i\ell_1} |k_1, k_2, \ell, \alpha\rangle, \quad T_2 |k_1, k_2, \ell, \alpha\rangle = e^{i\ell_2} |k_1, k_2, \ell, \alpha\rangle \tag{D4} $$

where $k_1 \in (-\pi, \pi)$ and we may choose $k_2 \in (-\pi/2, \pi/2)$. Note that these eigenstates differ from the conventional “momentum” eigenstates in Eq. (A40) which were used to diagonalize the Hofstadter Hamiltonian in App. [A]. Now we can form the Hofstadter Hamiltonian $H^{\Phi/2}(k)$ in this magnetic translation operator eigenbasis directly:

$$ H_{\ell_1, \ell_2}^{\Phi/2}(k)\delta_{k,k'} = (k_1, k_2, \ell, \alpha |H^{\Phi/2}|k_1, k_2, \ell, \beta\rangle, \quad k_1 \in (-\pi, \pi), k_2 \in (-\pi/2, \pi/2) \tag{D5} $$
due to Eq. (D8), the spectrum is invariant under closing proof in Sec. by choosing the half magnetic BZ defined by 

$$ U \times H - V $$

fall in generated under the application of $U^T$ and $V_1(\Phi/2)$. We denote these points with dots, and observe that exactly two points fall in $BZ_{1/2, \mathbf{k}}$.

which gives a representation of the Hamiltonian in the $1 \times 2$ unit cell. We emphasize that the states Eq. (D4) give the minimal, gauge-independent $1 \times 2$ unit cell, but we do not have an explicit expression for the Hofstadter Hamiltonian. We can derive the embedding matrices for $\mathcal{H}^{\Phi/2}(\mathbf{k})$ that implement the $k_1 \to k_1 + \pi$ periodicity following Sec. . We prove in App. D 2 b that there is an embedding matrix $[V_1(\Phi/2, k_2)]_{\ell,\alpha,\ell',\beta}$ satisfying 

$$ \mathcal{H}^{\Phi/2}(\mathbf{k} + \pi \mathbf{b}_1) = V_1(\Phi/2, k_2) \mathcal{H}^{\Phi/2}(\mathbf{k}) V_1^\dagger(\Phi/2, k_2). $$

We will not need an explicit expression for $V_1(\Phi/2, k_2)$ in this section, but we provide one in App. D 2 b. Note that this embedding matrix depends on $k_2$, which we make explicit in the notation. This differs from the embedding matrices in App. A 8 where there was no momentum dependence.

So far we have constructed the Hofstadter Hamiltonian in a gauge-invariant manner that guarantees a magnetic BZ, shown with an “X” is invariant under $U^T$ symmetry that protects a $\mathbb{Z}_2$ index, recalling that $(U^T)^2 = T^2 = -1$. We need to determine what properties this symmetry enforces. We will prove in App. D 2 b that

$$ \sum_{\ell',\alpha,\ell',\beta} |D(U^T)|_{\ell,\alpha,\ell',\beta} \mathcal{H}^{\Phi/2}(\mathbf{k}) |D(U^T)|_{\ell',\alpha',\ell',\beta'} = \mathcal{H}^{\Phi/2}(-\mathbf{k} - \mathbf{\kappa}) $$

where $D(U^T)$ is the representation of $U^T$ on the single-particle Hilbert space satisfying $D(U^T)[D(U^T)]^* = -1$ and $\mathbf{\kappa}$ is a momentum shift. We give a formula for $\mathbf{\kappa}$ in App. D 2 b where we show that it appears as a projective phase in the magnetic space group.

In Sec. of the Main Text, we proved that the $\mathbb{Z}_2$ invariant was always trivial, $\delta^{\Phi=\Phi/2} = +1$, for $\Phi = 2\pi n$, $n$ odd when $\mathbf{\kappa} = 0$ by proving that all gap closings come in pairs in the half magnetic BZ. To prove the case with arbitrary $\mathbf{\kappa}$, we note that we can rewrite Eq. (D7) in terms of a shifted momentum $\mathbf{k} = -\mathbf{\kappa} + \tilde{\mathbf{k}}$. In matrix notation, this reads

$$ D(U^T)^\dagger \mathcal{H}^{\Phi/2}(-\frac{1}{2}\mathbf{\kappa} + \tilde{\mathbf{k}}) D(U^T) = \mathcal{H}^{\Phi/2}(-\frac{1}{2}\mathbf{\kappa} - \tilde{\mathbf{k}}) $$

from which we observe that $\tilde{\mathbf{k}}$, the momentum measured from $-\frac{1}{2}\mathbf{\kappa}$, flips sign under $U^T$. Thus we can replicate the gap closing proof in Sec. by choosing the half magnetic BZ defined by $BZ_{1/2, \mathbf{k}} = \{-\frac{1}{2}\mathbf{\kappa} + \tilde{\mathbf{k}} | k_1 \in (-\pi, 0), \tilde{k}_2 \in (-\pi/2, \pi/2)\}$. Now we use the fact that $n$ is odd, so there is a $\pi$ periodicity in the spectrum along $k_1$ given by Eq. (D6). In addition, due to Eq. (D8), the spectrum is invariant under $\mathbf{k} \to -\mathbf{k} - \mathbf{\kappa}$. Hence gap closings in the whole magnetic BZ come in quartets, two due to the magnetic translation group and two due to $U^T$, at the points 

$$ -\frac{1}{2}\mathbf{\kappa} + \mathbf{b}_1, -\frac{1}{2}\mathbf{\kappa} - \mathbf{b}_1, -\frac{1}{2}\mathbf{\kappa} + \mathbf{\kappa} + \mathbf{b}_1, \text{ and } -\frac{1}{2}\mathbf{\kappa} - \mathbf{\kappa} + \mathbf{b}_1 $$

as is shown for instance in Fig. 12. Note that for generic $\mathbf{k}$, exactly one of $-\frac{1}{2}\mathbf{\kappa} \pm \mathbf{k}$ is in $BZ_{1/2, \mathbf{k}}$ and similarly exactly one of $-\frac{1}{2}\mathbf{\kappa} \mp \mathbf{b}_1$ is in $BZ_{1/2, \mathbf{k}}$. The degenerate points with $k_1 = 0, \pm \pi/2$ or $\pi$ and $k_2 = 0$ or $\pi/2$ reduce the quartet of points in Eq. (D9) to pairs of points where doubly degenerate gap closings occur. Thus all gap closings in the half BZ, $BZ_{1/2, \mathbf{k}}$, come in pairs and $\delta^{\Phi=\Phi/2} = +1$. 

FIG. 12. We illustrate an example of $BZ_{1/2, \mathbf{k}}$, shown in red, with the rest of the magnetic BZ shown in blue. The point $-\mathbf{\kappa}/2$, shown with an “X” is invariant under $U^T$. If there is a gap closing at $k = -\frac{1}{2}\mathbf{\kappa} + \mathbf{k}$, then three more gap closings are generated under the application of $U^T$ and $V_1(\Phi/2)$. We denote these points with dots, and observe that exactly two points fall in $BZ_{1/2, \mathbf{k}}$. 

[Diagram of BZ with arrows and points indicating gap closings]
b. Construction of the Gauge-invariant Eigenstates and the Projective Symmetry Algebra

To compute objects like $T_i |\beta, \ell', k_1, k_2\rangle$ and $U T |\beta, \ell', k_1, k_2\rangle$, we note that there is an explicit expression for the momentum eigenstates given by the magnetic translation operators

$$|k_1, k_2, \ell, \alpha\rangle = \frac{1}{\sqrt{N/2}} \sum_{mn} e^{-imk_1 - 2imk_2 T_1^m T_2^{2n} T_2^{\dagger}_{m,n} c_{\alpha_{m,n}},} |0\rangle , \quad \ell = 0, 1 \text{ and } \alpha = 1, \ldots, N_{\text{orb}}$$

(D10)

where $T_i^{-m} = [T_i^m]^m$. (Recall that have have denoted $T_i (\Phi/2)$ as $T_i$ for brevity). It is straightforward to check that these states have the correct $T_1, T_2^2$ eigenvalues. Here we have assumed $n$ odd so there is a $1 \times 2$ magnetic unit cell. We will first use Eq. (D10) to derive the embedding matrix $V_1 (\Phi/2, k_2)$ (see Eq. (D6)). We treat the cases of $\ell = 0$ and $\ell = 1$ separately. For $\ell = 0$, we find

$$T_2 |k_1, k_2, 0, \alpha\rangle = \frac{1}{\sqrt{N/2}} \sum_{mn} e^{-imk_1 - 2imk_2 T_1^m T_2^{2n} T_2^{\dagger}_{m,n} c_{\alpha_{m,n}},} |0\rangle$$

$$= \frac{1}{\sqrt{N/2}} \sum_{mn} e^{-imk_1 - 2imk_2 (-1)^m T_1^m T_2^{2n} T_2^{\dagger}_{m,n} c_{\alpha_{m,n}},} |0\rangle$$

$$= \frac{1}{\sqrt{N/2}} \sum_{mn} e^{-im(k_1 + \pi) - 2imk_2 T_1^m T_2^{2n} T_2^{\dagger}_{m,n} c_{\alpha_{m,n}},} |0\rangle$$

(D11)

using the magnetic translation group and $\exp(i \Phi/2) = -1$ for $n$ odd. Now using Eq. (A9) to compute the action of $T_2$ on the single-particle state, we find

$$T_2 c_{\alpha_{m,n},}^{\dagger} |0\rangle = \exp \left( i \int_{\delta_\alpha} A \cdot d\mathbf{r} + i \chi_2 (\delta_\alpha) \right) c_{\alpha_{m,n},}^{\dagger} |0\rangle$$

(D12)

and hence

$$T_2 |k_1, k_2, 0, \alpha\rangle = \exp \left( i \int_{\delta_\alpha} A \cdot d\mathbf{r} + i \chi_2 (\delta_\alpha) \right) |k_1 + \pi, k_2, 1, \alpha\rangle$$

(D13)

For $\ell = 1$, we calculate

$$T_2 |k_1, k_2, 1, \alpha\rangle = \frac{1}{\sqrt{N/2}} \sum_{mn} e^{-imk_1 - 2imk_2 T_1^m T_2^{2n+1} T_2^{\dagger}_{m,n} c_{\alpha_{m,n},}^{\dagger}} |0\rangle$$

$$= \frac{1}{\sqrt{N/2}} \sum_{mn} e^{-im(k_1 + \pi) - 2imk_2 T_1^m T_2^{2n+1} T_2^{\dagger}_{m,n} c_{\alpha_{m,n},}^{\dagger}} |0\rangle$$

$$= \frac{1}{\sqrt{N/2}} \sum_{mn} e^{-im(k_1 + \pi) - 2imk_2 T_1^m T_2^{2n+2} T_2^{\dagger}_{m,n} c_{\alpha_{m,n},}^{\dagger}} |0\rangle$$

$$= \frac{1}{\sqrt{N/2}} \sum_{mn} e^{-im(k_1 + \pi) - 2im(k_2 - 1)k_2 T_1^m T_2^{2n+2} T_2^{\dagger}_{m,n} c_{\alpha_{m,n},}^{\dagger}} |0\rangle$$

(D14)

Now using Eq. (A9) to compute the action of $T_2^{\dagger}$ on the single-particle state, we find

$$T_2^{\dagger} c_{\alpha_{m,n},}^{\dagger} |0\rangle = \exp \left( -i \int_{\delta_\alpha} A \cdot d\mathbf{r} - i \chi_2 (\delta_\alpha) \right) c_{\alpha_{m,n},}^{\dagger} |0\rangle$$

(D15)

and hence

$$T_2 |k_1, k_2, 1, \alpha\rangle = \exp \left( 2ik_2 - i \int_{\delta_\alpha} A \cdot d\mathbf{r} - i \chi_2 (\delta_\alpha) \right) |k_1 + \pi, k_2, 0, \alpha\rangle .$$

(D16)

We collect Eqs. (D13) and (D16) into the following formula

$$T_2 |k_1, k_2, \ell, \alpha\rangle = \sum_{\ell', \beta} |k_1 + \pi, k_2, \ell', \beta\rangle [V_1 (\Phi/2, k_2)]_{\ell', \beta, \ell, \alpha}$$

(D17)
where

\[ [V_1(\Phi/2, k_2)]_{\ell', \ell} = \delta_{\ell, \ell'} e^{ik_2} \left[ \cos \left( k_2 - \int_{\delta_\alpha}^{\alpha+\delta_\alpha} A \cdot dr - \chi_2(\delta_\alpha) \right) \right]_1 + \sin \left( k_2 - \int_{\delta_\alpha}^{\alpha+\delta_\alpha} A \cdot dr - \chi_2(\delta_\alpha) \right) \right]_2 \]

(D18)

which by inspection is a unitary matrix. We remark that \( V_1(\Phi/2, k_2) \) is periodic along the magnetic BZ, i.e. \( V_1(\Phi/2, k_2) = V_1(\Phi/2, k_2 - \pi) \), which we will make use of in App. D3a when considering the Wilson loop. We derive the corresponding transformation on the Hofstadter Hamiltonian to be

\[ \mathcal{H}^{\Phi/2}_{\ell, \alpha, r, \beta}(k_1, k_2) = \sum_{\ell', \alpha', \beta'} \left[ V_1(\Phi/2, k_2) \right]_{\ell, \ell'} \mathcal{H}^{\Phi/2}_{\ell', \alpha', r, \beta'}(k_1 + \pi, k_2) \]

(D19)

In matrix notation, this reads

\[ \mathcal{H}^{\Phi/2}(k) = V_1(\Phi/2, k_2) \mathcal{H}^{\Phi/2}(k + \pi b_1) V_1(\Phi/2, k_2) \]

(D20)

which proves Eq. [D6].

In a similar manner, we can compute the action of \( UT \) on the eigenstates Eq. (D10) once we know the algebra of \( UT \) and \( T_1(\Phi/2) \). Using Eq. (A9), we compute

\[ T T_1(\Phi/2) T^{-1} = \sum_{R \alpha} e^{i \int_{R+\delta_\alpha}^{R+\delta_\alpha} A \cdot dr + i R \chi(R + \delta_\alpha)} c_{R+\delta_\alpha, \alpha} c_{R, \alpha} T^{-1} \]

(D21)

where the integral of \( A \) is taken over a straight-line path, which is not necessarily a Peierls path. Using Eq. (D2), we compute

\[ T T_1(\Phi/2) T^{-1} = \sum_{R \alpha} e^{-i \int_{R+\delta_\alpha}^{R+\delta_\alpha} A \cdot dr - i R \chi(R + \delta_\alpha)} c_{R+\delta_\alpha, \alpha} c_{R, \alpha} T^{-1} \]

= \[ \sum_{R \alpha, \alpha', \alpha''} e^{-i \int_{R+\delta_\alpha}^{R+\delta_\alpha} A \cdot dr - i R \chi(R + \delta_\alpha)} c_{R+\delta_\alpha, \alpha} D_{\alpha', \alpha''}^{\alpha}(T) D_{\alpha''}^{\alpha'}(T) c_{R, \alpha''} \]

(D22)

where we have used the fact that \( T \) is onsite as discussed in App. D1. We see that the effect of \( T \) is merely to complex conjugate \( T_1(\phi) \), which is equivalent to reversing the flux. We now study \( U T T_1(\phi)(U T)^{-1} = U T_1(-\phi) U^\dagger \). Using Eq. (A5), we find

\[ U T_1(-\Phi/2) U^\dagger = \sum_{R \alpha} e^{-i \int_{R+\delta_\alpha}^{R+\delta_\alpha} A \cdot dr - i R \chi(R + \delta_\alpha)} U c_{R+\delta_\alpha, \alpha} U^\dagger \]

= \[ \sum_{R \alpha} \exp \left( -i \int_{R+\delta_\alpha}^{R+\delta_\alpha} A \cdot dr - i R \chi(R + \delta_\alpha) + i \int_{R_0}^{R+\delta_\alpha} \tilde{A} \cdot dr - i \int_{R_0}^{R+\delta_\alpha} \tilde{A} \cdot dr \right) \]

(D23)

where we emphasize that the integral of \( \tilde{A} \) (generating \( \Phi \) flux) is taken over a Peierls path (see Eq. (2c)) and the integral of \( A \) (generating \( \phi = \Phi/2 \) flux) is taken over a straight-line path (see Eq. (3)). We can re-sum the Peierls integrals using Eq. (A4)

\[ U T_1(-\Phi/2) U^\dagger = \sum_{R \alpha} \exp \left( -i \int_{R+\delta_\alpha}^{R+\delta_\alpha} A \cdot dr - i R \chi(R + \delta_\alpha) + i \int_{R_0}^{R+\delta_\alpha} \tilde{A} \cdot dr \right) \]

(D24)

To proceed, we want to relate the gauge fields \( A \) and \( \tilde{A} \) in a convenient way. We have \( 2A = \tilde{A} \) up to a gauge transformation because \( \nabla \times A = \Phi/2 \) and \( \nabla \times \tilde{A} = \Phi \). It is most convenient to take \( 2A = \tilde{A} \). We now note that the integrals can be combined. For clarity, we denote integrals over Peierls paths with a P.P. label, and the straight-line path with straight, and we also denote \( \mathbf{R} + \delta_\alpha = \mathbf{r}_\alpha \) as shorthand. Then the integrals in Eq. (D24) can be manipulated...
depict in Fig. 13a. Importantly, the Peierls paths connecting consider a closed loop \( \partial \tilde{A} \).

To prove Eq. (D31), we recall that any integral of \( \tilde{A} \) is over a loop given by a Peierls path from \( \mathbf{r}_\alpha \) to \( \mathbf{r}_\alpha + \mathbf{a}_i \) (which may be taken along an arbitrary sequence of Peierls paths because \( \nabla \times \tilde{A} = \Phi \)) and then a straight-line path back from \( \mathbf{r}_\alpha + \mathbf{a}_i \) to \( \mathbf{r}_\alpha \). We denote the area enclosed by such a path as \( \Omega_{i,\alpha} \), as shown for example in Fig. 13a. Continuing, we find

\[
-\int_{\text{straight}}^{\mathbf{r}_\alpha \rightarrow \mathbf{r}_\alpha + \mathbf{a}_i} \mathbf{A} \cdot d\mathbf{r} = \int_{\text{straight}}^{\mathbf{r}_\alpha \rightarrow \mathbf{r}_\alpha + \mathbf{a}_i} \tilde{\mathbf{A}} \cdot d\mathbf{r} = \int_{\text{straight}}^{\mathbf{r}_\alpha \rightarrow \mathbf{r}_\alpha + \mathbf{a}_i} \mathbf{A} \cdot d\mathbf{r} = \int_{\text{straight}}^{\mathbf{r}_\alpha \rightarrow \mathbf{r}_\alpha + \mathbf{a}_i} \tilde{\mathbf{A}} \cdot d\mathbf{r} - 2\int_{\text{straight}}^{\mathbf{r}_\alpha \rightarrow \mathbf{r}_\alpha + \mathbf{a}_i} \mathbf{A} \cdot d\mathbf{r} + \int_{\text{straight}}^{\mathbf{r}_\alpha \rightarrow \mathbf{r}_\alpha + \mathbf{a}_i} \tilde{\mathbf{A}} \cdot d\mathbf{r} \quad (D25)
\]

and thus we find

\[
UT_i(\Phi/2)U^\dagger = \sum_{\mathbf{R}_\alpha} \exp \left( i\Phi_{i,\alpha} + i \int_{\mathbf{R} + \delta_{\alpha} + \mathbf{a}_i}^{\mathbf{R} + \delta_{\alpha}} \mathbf{A} \cdot d\mathbf{r} - i\chi_i(\mathbf{R} + \delta_{\alpha}) \right) c_{\mathbf{R} + \delta_{\alpha} + \mathbf{a}_i}^{\dagger} c_{\mathbf{R} + \delta_{\alpha}}. \quad (D27)
\]

We want to recover an expression proportional to the magnetic translation operator \( T_i(\Phi/2) \). To make progress, we note that at \( \phi = \Phi/2 \), Eq. (A9) gives \( \chi_i(\mathbf{r}) = \Phi/2(\mathbf{a}_i \times \mathbf{r}) \) and hence

\[
-\chi_i(\mathbf{R} + \delta_{\alpha}) = \chi_i(\mathbf{R} + \delta_{\alpha}) - \Phi \mathbf{a}_i \times (\mathbf{R} + \delta_{\alpha}) = \chi_i(\mathbf{R} + \delta_{\alpha}) - \Phi \mathbf{a}_i \times \delta_{\alpha} \quad \text{mod } 2\pi \quad (D28)
\]

and hence

\[
UT_i(\Phi/2)U^\dagger = \sum_{\mathbf{R}_\alpha} \exp \left( i\Phi_{i,\alpha} + \delta_{\alpha} \times \mathbf{a}_i \right) c_{\mathbf{R} + \delta_{\alpha} + \mathbf{a}_i}^{\dagger} c_{\mathbf{R} + \delta_{\alpha}}. \quad (D29)
\]

We can now define the momentum shift \( \kappa \) by

\[
\kappa_{i,\alpha} = \Phi(\Omega_{i,\alpha} + \delta_{\alpha} \times \mathbf{a}_i). \quad (D30)
\]

It appears that the momentum shift depends on the orbital location. However, we will now prove that, in fact

\[
\kappa_{i,\alpha} - \kappa_{i,\beta} = \Phi(\Omega_{i,\alpha} - \Omega_{i,\beta} + (\delta_{\alpha} - \delta_{\beta}) \times \mathbf{a}_i) = 0 \quad \text{mod } 2\pi \quad (D31)
\]

To prove Eq. (D31), we recall that any integral of \( \tilde{A} \) over a closed loop of Peierls paths is equal to a multiple of \( 2\pi \). We consider a closed loop \( \partial \mathcal{M} \) that is formed of Peierls paths connecting \( \delta_{\alpha} + \mathbf{a}_i, \delta_{\beta} + \mathbf{a}_i, \delta_{\beta} + \mathbf{a}_i \) in sequence, which we depict in Fig. 13a. Importantly, the Peierls paths connecting \( \delta_{\alpha}, \delta_{\beta} \) and \( \delta_{\alpha} + \mathbf{a}_i, \delta_{\beta} + \mathbf{a}_i \) can be chosen to be the same shape since they are related by a lattice vector. Now, as shown in Fig. 13a we can separate the line integral over \( \partial \mathcal{M} \) with straight-line paths connecting \( \delta_{\alpha}, \delta_{\alpha} + \mathbf{a}_i \) and \( \delta_{\beta}, \delta_{\beta} + \mathbf{a}_i \):

\[
0 = \int_{\partial \mathcal{M}} \tilde{A} \cdot d\mathbf{r} \quad \text{mod } 2\pi
\]

\[
= \int_{\partial \Omega_{i,\alpha}} \tilde{A} \cdot d\mathbf{r} + \int_{\partial \Omega_{i,\beta}} \tilde{A} \cdot d\mathbf{r} + \int_{-\partial \Omega_{i,\beta}} \tilde{A} \cdot d\mathbf{r} \quad \text{mod } 2\pi
\]

\[
= \Phi \int_{\Omega_{i,\alpha}} d\mathbf{S} + \Phi \int_{\Omega_{i,\beta}} d\mathbf{S} - \Phi \int_{\Omega_{i,\beta}} d\mathbf{S} \quad \text{mod } 2\pi
\]

\[
= \Phi(\Omega_{i,\alpha} - \Omega_{i,\beta}) + \Phi \int_{\partial} d\mathbf{S} \quad \text{mod } 2\pi
\]
Now assuming $U$ we remark that this result, the algebra of proving Eq. (D31). Hence we can calculate $\kappa \kappa \kappa$ changing its area. Hence the area of $\delta \delta \delta$ and $\alpha \alpha \alpha$ where $R$ is due to the opposite orientation. We see and can easily prove that $\mathcal{R}$ can be deformed to a parallelogram with corners at $\delta \delta \delta, \delta \delta \delta + a_2, \delta \delta \delta + a_2$, and $\delta \delta \delta$.

where $\mathcal{R}$, shown in Fig. 13c, is the area formed by the straight-line paths and the Peierls paths connecting $\delta \delta \delta, \delta \delta \delta + a_1, \delta \delta \delta + a_1, \delta \delta \delta + a_1$. Because these Peierls paths are the same shape, $\mathcal{R}$ can be deformed to a parallelogram without changing its area. Hence the area of $\mathcal{R}$ is that of a parallelogram with sides given by $a_1$ and $\delta \delta \delta - \delta \delta \delta$. Thus, Eq. (D32) reads

$$\Phi(\Omega_{i,\delta} - \Omega_{i,\beta}) + a_i \times (\delta \delta \delta - \delta \delta \delta) = 0 \mod 2\pi,$$

proving Eq. (D31). Hence we can calculate $\kappa = \kappa \alpha$ at any orbital location. However, we must be consistent with the choice of origin which defines $\delta \delta \delta$. Shifting the origin changes both $\kappa$ and the overall phase of $T_i(\Phi/2)$, which we have fixed throughout. Note however that Eq. (D31) remains invariant under such a shift.

With $\kappa = \kappa_1 \beta_1 + \kappa_2 \beta_2$ determined, we return to Eq. (D29) to obtain

$$UTT_i(\Phi/2)(UT)^{-1} = \left[ \sum_{R_{10}} \exp \left( ik_i + i \int_{R+\delta_\alpha+a_1} A \cdot dr + i \chi_i(R+\delta_\alpha) \right) c^{\dagger}_{R+\alpha,\alpha} c_{R,\alpha} \right]$$

We remark that this result, the algebra of $UT$ and $T_i(\Phi/2)$ holds for $n$ even or odd, and regardless of the sign of $T^2$. Now assuming $n$ odd so there is a $1 \times 2$ unit cell, (Eq. (D34)) lets us calculate

$$UT |k_1,k_2,\ell,\alpha\rangle = \frac{1}{\sqrt{N/2}} \sum_{m_1} e^{+im_1k_1 + 2imk_2} UTT_1T_2^{m_1} T_2^{m_2} (UT)^{-1} UT c^{\dagger}_{\alpha_1,\alpha_2} |0\rangle$$

$$(D35)$$

where in the last line we defined $D^1(UT)$, the single-particle representation of $UT$ (with $K$ denoting complex conj
This follows from
\[ U T_c^i \left| a_{\alpha}, 0 \right\rangle = U T_{c_{a_{\alpha}}} T^{-1} U T \left| 0 \right\rangle = U T_{c_{a_{\alpha}}} T^{-1} U \left| 0 \right\rangle K \]
\[ = \sum_{\alpha'} U T_{c_{a_{\alpha}}} U \left[ D_{\alpha \alpha'} (T) \right] \left| 0 \right\rangle K \]
\[ = \sum_{\alpha', \alpha} c_{a_{\alpha}, a_{\alpha'}} \delta_{\alpha \alpha'} e^{i \delta_{\alpha \alpha'} } \tilde{A} \delta \left| 0 \right\rangle K D_{\alpha \alpha'} (T) \]
\[ = \sum_{\alpha', \alpha} c_{a_{\alpha}, a_{\alpha'}} \left| 0 \right\rangle \delta_{\alpha \alpha'} e^{-i \delta_{\alpha \alpha'} } \tilde{A} \delta D_{\alpha \alpha'} (T) \]
\[ = \sum_{\alpha', \alpha} c_{a_{\alpha}, a_{\alpha'}} \left| 0 \right\rangle \left[ D^{\dagger} (U T) \right]_{\alpha', \alpha} \delta_{\alpha \alpha'} \left[ D (U T) \right]_{\alpha' \alpha} = \delta_{\alpha \alpha'} e^{-i \delta_{\alpha \alpha'} } \tilde{A} \delta D_{\alpha \alpha'} (T) \]

with \( \ell = 0, 1 \) and \( \alpha = 1, \ldots, N_{\text{orb}} \) in a tensor product basis.

To determine the action of \( U T \) on the Hofstadter Hamiltonian, we use the fact that \( U T \) commutes with \( H^{\Phi/2} \), giving
\[ \mathcal{H}^{\Phi/2}_{\ell \alpha, \ell' \beta} (k) = \sum_{\ell \alpha', \ell' \beta'} \left[ D (U T) \right]_{\ell \alpha, \ell' \alpha'} \mathcal{H}^{\Phi/2}_{\ell' \alpha', \ell' \beta'} (k) \mathcal{H}^{\Phi/2}_{\ell' \alpha', \ell' \beta'} (-k - \kappa) \left[ D^{\dagger} (U T) \right]_{\ell' \beta', \ell' \beta} . \]  

We recognize the usual form of an anti-unitary symmetry acting on a single-particle Hamiltonian, but with a momentum shift that comes from the algebra of \( U T \) and \( T (\Phi/2) \). We mention that the full symmetry algebra of \( H^{\Phi/2} \),
\[ UT, T_1 (\Phi/2) \]
forms a projective representation of the magnetic space group \( 1' \) at \( \phi = 0 \) with the projective phases \( \phi \) and \( \kappa \) given by
\[ T_1 (\Phi/2) T_2 (\Phi/2) = e^{i \Phi/2} T_2 (\Phi/2) T_1 (\Phi/2), \]
\[ U T T_1 (\Phi/2) = e^{i \kappa \cdot b} T_1 (\Phi/2) T_1 (\Phi/2) \] .

For instance, we can consider the model of twisted bilayer graphene introduced in App. [G1]. In Fig. [13] we show that, due to the Peierls paths being taken through the center of the honeycomb, we find nonzero expression for \( \Omega_{\ell \alpha} \). Choosing a convention where the origin is fixed at the center of the honeycomb, we find that Eq. [D30] yields \( \kappa = (\pi, \pi) \).

### 3. Wilson Loop Proof of a Nontrivial \( \mathbb{Z}_2 \) Index with \( T \) symmetry

The crux of our proof in Sec. is the establishment that the \( \mathbb{Z}_2 \) Kane-Mele invariant of \( H^{\Phi/2} \) is trivial. App. [D2] demonstrated this using the action of the magnetic translation group on the BZ. Here, we prove the same result using the Wilson loop. We assume that the magnetic periodicity is given \( \Phi = 2 \pi n, n \) odd and we will prove that \( \delta_{\phi = 2 \pi} = +1 \). In App. [F2] we show when \( n \) is even, \( \delta_{\phi = 2 \pi} \) is not fixed to be +1.

#### a. \( U T \) Constraints on the Wilson Loop

To begin, we study the constraint imposed by \( U T \) on the Wilson loop at \( \phi = \Phi/2 \) in the \( 1 \times 2 \) gauge-invariant magnetic unit cell. To begin, we need to work in an eigenbasis of \( H^{\Phi/2}, T_1 (\Phi/2), T_2^2 (\Phi/2) \) which is given by
\[ |m, k\rangle = \sum_{\ell \alpha} |k, \ell, \alpha\rangle |u^{\ell \alpha} (k)|_{\ell \alpha, m}, \quad \ell = 0, 1 , \alpha = 1 , \ldots , N_{\text{orb}}, \; \text{and} \; m = 1 , \ldots , 2 N_{\text{orb}} \]

where \( |u^{\ell \alpha} (k)|_{\ell \alpha, m} \) is a \( 2 N_{\text{orb}} \times 2 N_{\text{orb}} \) unitary matrix which relates the \( \ell, \alpha \) basis (in Eq. [D4]) to the \( m \) energy eigenbasis of \( \mathcal{H}^{\Phi/2} (k) \). To follow the method of App. [C1] we write define \( |u^{\Phi/2} (k)\rangle \), the eigenstate of \( \mathcal{H}^{\Phi/2} (k) \), by
\[ (k, \ell, \alpha | u^{\Phi/2} (k) \rangle = |U(k)|_{\ell \alpha, j} \]

\[ (k, \ell, \alpha | u^{\Phi/2} (k) \rangle) = |U(k)|_{\ell \alpha, j} \]
Using Eq. (D45), we find \( \tilde{\delta}_k \). We now want to consider a full Wilson loop. Because of the shift due to the path in dashed black for a given orbital \( \delta_\alpha \), we find \( \Phi \) is defined as in Eq. (D30), we find \( \delta_\beta \). We recall that \( \Phi = 6\pi \), as discussed in detail in App. [G1], so \( \Phi \Omega_{\alpha,\alpha} = \pi \). In the convention where the origin is at the center of the honeycomb, we calculate \( \Phi \delta_\alpha \times a_1 = 6\pi(-\delta_{1/2} + a_1/2) \times a_1 = 6\pi \times 1/3 = 0 \mod 2\pi \), and hence from Eq. (D30), we find \( \kappa_1 = \pi \). (c) We show the area \( \Omega_{\alpha,\beta} = 1/6 \) enclosed by the Peierls Paths (shown in solid blue) and the straight-line path in dashed black for a given orbital \( \delta_\beta \). We recall that \( \Phi = 6\pi \), as discussed in detail in App. [G1] so \( \Phi \Omega_{\alpha,\beta} = \pi \). In the convention where the origin is at the center of the honeycomb, we calculate \( \Phi \delta_\beta \times a_2 = 6\pi(-\delta_{1/2} - a_1/2) \times a_2 = 6\pi \times -2/3 = 0 \mod 2\pi \), and hence from Eq. (D30), we find \( \kappa_2 = \pi \).

where \( j = 1, \ldots, 2N_{\text{occ}} \), assuming the energy spectrum is gapped for \( \phi \in (0, \Phi/2) \) and we can separate the occupied bands. For convenience, we define the unitary matrix \( Q = \mathcal{D}(UT) \) which, by Eq. (D7), satisfies

\[
Q K \mathcal{H}^{\Phi/2}(k) K^\dagger = \mathcal{H}^{\Phi/2}(-k - \kappa)
\]

where \( K \) is complex conjugation. Following App. [CT] we now form the unitary sewing matrix

\[
B_{ij}^\Phi = \langle u_i^{\Phi/2}(-k - \kappa)|QK|u_j^{\Phi/2}(k)\rangle = \langle u_i^{\Phi/2}(-k - \kappa)|Q|u_j^{\Phi/2,*}(k)\rangle
\]

which connects eigenstates at TRS momenta \( \kappa \).

Using this relation, we determine that a small segment of a Wilson loop obeys

\[
[W_k^{\Phi/2}]_{ij} = \langle u_i^{\Phi/2}(k)|u_j^{\Phi/2}(k)\rangle = \sum_r B_{ij}^{\Phi/2,r} \langle u_r^{\Phi/2,*}(-k - \kappa)|Q|u_r^{\Phi/2,*}(-k - \kappa)\rangle |B_{ij}^{\Phi/2}|^2
\]

We now want to consider a full Wilson loop. Because of the shift due to \( \kappa \), we will find it convenient to shift the origin of the Wilson loop. Hence we define \( \hat{k} \) by \( k = -\kappa/2 + \hat{k} \) and define a Wilson loop \( \tilde{W}^{\Phi/2}(\hat{k}_1) \) by integrating along \( \hat{k}_2 \):

\[
\tilde{W}^{\Phi/2}(\hat{k}_1) \equiv \prod_{(\kappa_1/2 + \hat{k}_1, -\kappa_2/2 + \pi/2)}^{(-\kappa_1/2 + \hat{k}_1, -\kappa_2/2 - \pi/2)} \prod_{(-\kappa_1/2 + \hat{k}_1, -\kappa_2/2 + \pi/2)} \tilde{W}^{\Phi/2} (\hat{k}_1)
\]

Using Eq. (D45), we find

\[
\tilde{W}^{\Phi/2}(\hat{k}_1) = B_{(-\kappa_1/2 + \hat{k}_1, -\kappa_2/2 + \pi/2)} \tilde{W}^{\Phi/2,*} (\hat{k}_1) B_{(-\kappa_1/2 + \hat{k}_1, -\kappa_2/2 + \pi/2)} = B_{(-\kappa_1/2 + \hat{k}_1, -\kappa_2/2 + \pi/2)} \tilde{W}^{\Phi/2,*} (\hat{k}_1) B_{(-\kappa_1/2 + \hat{k}_1, -\kappa_2/2 + \pi/2)}
\]

FIG. 14. (a) We show the lattice vectors and nearest neighbor vectors of the TBG model, replicated from Fig. [8]. (b) We show the area \( \Omega_{\alpha,\alpha} = 1/6 \) enclosed by the Peierls Paths (shown in solid red) and the straight-line path in dashed black for a given orbital \( \delta_\alpha \). We recall that \( \Phi = 6\pi \), as discussed in detail in App. [G1], so \( \Phi \Omega_{\alpha,\alpha} = \pi \). In the convention where the origin is at the center of the honeycomb, we calculate \( \Phi \delta_\alpha \times a_1 = 6\pi(-\delta_{1/2} + a_1/2) \times a_1 = 6\pi \times 1/3 = 0 \mod 2\pi \), and hence from Eq. (D30), we find \( \kappa_1 = \pi \). (c) We show the area \( \Omega_{\alpha,\beta} = 1/6 \) enclosed by the Peierls Paths (shown in solid blue) and the straight-line path in dashed black for a given orbital \( \delta_\beta \). We recall that \( \Phi = 6\pi \), as discussed in detail in App. [G1] so \( \Phi \Omega_{\alpha,\beta} = \pi \). In the convention where the origin is at the center of the honeycomb, we calculate \( \Phi \delta_\beta \times a_2 = 6\pi(-\delta_{1/2} - a_1/2) \times a_2 = 6\pi \times -2/3 = 0 \mod 2\pi \), and hence from Eq. (D30), we find \( \kappa_2 = \pi \).
We now observe that from the construction of the translation eigenstates in Eq. (D10), we have \( |k_1, k_2, \ell, \alpha\rangle = |k_1 + 2\pi, k_2, \ell, \alpha\rangle \), and thus from Eq. (D5), we find that \( \mathcal{H}^{\Phi/2}(k_1, k_2) = \mathcal{H}^{\Phi/2}(k_1 + 2\pi, k_2) \). In other words, the embedding matrices that enforce the magnetic BZ periodicity are trivial. This is due to the choice of the eigenbasis in Eq. (D10), which differ from the bases we considered in Eq. (A40) in the Landau gauge. Hence, we have

\[
\mathcal{B}^{ij}_{(-\kappa_1/2-k_1,-\kappa_2/2+\pi/2)} = \mathcal{B}^{ij}_{(-\kappa_1/2-k_1,-\kappa_2/2-\pi/2)} .
\]

(D48)

Returning to Eq. (D47) with this result, we find

\[
\tilde{W}^{\Phi/2}(\tilde{k}_1) = \mathcal{B}_{(-\kappa_1/2-k_1,-\kappa_2/2-\pi/2)} [\tilde{W}^{\Phi/2}(\tilde{k}_1)]^T \mathcal{B}_{(-\kappa_1/2-k_1,-\kappa_2/2-\pi/2)} .
\]

(D49)

We define the eigenvalues of \( \tilde{W}^{\Phi/2}(\tilde{k}_1) \) as \( \exp i\hat{\vartheta}_j(\tilde{k}_1) \). Using Eq. (D49), we find the usual constraint on the Wannier centers:

\[
\{ \hat{\vartheta}_j(\tilde{k}_1) \} = \{ \hat{\vartheta}_j(-\tilde{k}_1) \}
\]

(D50)

emphasizing that \( \tilde{k}_1 \) is the coordinate measured from \(-\kappa/2\), i.e. \( \hat{\vartheta}_j(\tilde{k}_1) \) is the Wilson eigenvalue of the loop at \(-\kappa/2 + \tilde{k}_1 b_1\). By re-centering the magnetic BZ around \(-\kappa/2\), we have found that the \( UT \) symmetry behaves like \( T \) at \( \phi = 0 \) on the shifted Wilson loop \( \tilde{W}(\tilde{k}_1) \). We now study the constraint on the Wilson loop spectrum due to the \( \Phi/2 \) periodicity of \( \tilde{k}_1 \) (recalling that we take \( n \) odd here). From Eq. (D6), we have

\[
V_1(\Phi/2,k_2)\mathcal{H}^{\Phi/2}(k)V_1^\dagger(\Phi/2,k_2) = \mathcal{H}^{\Phi/2}(k + \pi b_1) .
\]

(D51)

Following App. C1 we now form the unitary sewing matrix

\[
B^{ij}_k = \langle u^\Phi_{j}(k + \pi b_1) | V_1(\Phi/2,k_2) | u^\Phi_{i}(k) \rangle
\]

(D52)

which is not to be confused with \( \mathcal{B}_k \), the sewing matrix for \( UT \) defined in Eq. (D43). \( B_k \) which connects eigenstates that are \( \pi b_1 \) apart [35]:

\[
| u^\Phi_{j}(k) \rangle = \sum_i V_1(\Phi/2,k_2) | u^\Phi_{i}(k + \pi b_1) \rangle [B^\dagger]^{ij}_k | \pi b_1 \rangle .
\]

(D53)

Following the same discussion in Eq. (D45), we find

\[
\tilde{W}^{\Phi/2}(\tilde{k}_1) = B_{(-\kappa_1/2+k_1+\pi,-\kappa_2/2+\pi/2)} \tilde{W}^{\Phi/2}(\tilde{k}_1 + \pi) B^\dagger_{(-\kappa_1/2+k_1+\pi,-\kappa_2/2-\pi/2)} .
\]

(D54)

The two embedding matrices \( B_{k} \) and \( B_{k-\pi b_2} \) are identical:

\[
B^{ij}_k = \langle u^\Phi_{i}(k + \pi b_1 - \pi b_2) | V_1(\Phi/2,k_2 - \pi) | u^\Phi_{j}(k - \pi b_2) \rangle = \langle u^\Phi_{i}(k + \pi b_1) | V_1(\Phi/2,k_2) | u^\Phi_{j}(k) \rangle
\]

(D55)

where we have used that the eigenstates (Eq. (D10)) and the embedding matrix \( V_1(\Phi/2,k_2) \) are periodic in \( \pi b_2 \), as we can see from App. D2b. Thus in the basis of Eq. (D10), we find that Eq. (D54) enforces

\[
\{ \hat{\vartheta}_j(\tilde{k}_1) \} = \{ \hat{\vartheta}_j(\tilde{k}_1 + \pi) \}
\]

(D56)

which is in contrast to Eq. (C12), which was performed in the Landau gauge. This is due to a different choice of eigenstates. In the Landau gauge, we chose to diagonalize the Hamiltonian in the basis of Eq. (A40) on which \( T_1(0) \) was diagonal (see App. A7). In contrast, the basis constructed in Eq. (D10) is diagonal under \( T_1(\Phi/2) \).

b. \( \mathbb{Z}_2 \) Index from the Wilson Loop

We will now see that, given Eqs. (D50) and (D56), the \( \mathbb{Z}_2 \) invariant must be trivial. Ref. [49] provides the following method of calculating \( \delta^{\Phi/2} \) from the Wilson loop eigenvalues. Draw an arbitrary line of arbitrary constant
$\tilde{\vartheta}(\tilde{k}_1) = \tilde{\vartheta}^\ast$ through the half Wilson spectrum $\{\tilde{\vartheta}_j(\tilde{k}_1)\}$, $\tilde{k}_1 \in (-\pi, 0)$ and count the number of times it crosses the Wilson bands; $\delta^{\phi=\Phi/2}$ is trivial if there are an even number of crossings, and non-trivial is there are are odd number. We emphasize $\tilde{k}$ refers to the momentum $k = -k/2 + \tilde{k}$ in the magnetic BZ. We will prove that all crossings of the Wilson loop spectrum with the arbitrary line $\tilde{\vartheta}$ occur in pairs, and hence $\delta^{\phi=\Phi/2}$ is trivial.

Suppose a crossing occurs at the point $(\tilde{k}_1^*, \tilde{\vartheta}^*)$ with $\tilde{k}_1^* \in (-\pi, 0)$, so there is a Wilson band satisfying $\tilde{\vartheta}(\tilde{k}_1^*) = \tilde{\vartheta}^*$. By $UT$, Eq. (D50) ensures there is also a band satisfying $\vartheta(-\tilde{k}_1^*) = \tilde{\vartheta}^*$. Then, using Eq. (D50), there are bars satisfying $\vartheta(-\tilde{k}_1^* - \pi) = \tilde{\vartheta}^*$ and $\vartheta(\tilde{k}_1^* + \pi) = \tilde{\vartheta}^*$. Note that generically, $\tilde{k}_1^*$ and $-\tilde{k}_1^* - \pi$ are distinct points and $-\tilde{k}_1^* - \pi \in (-\pi, 0)$ (see Fig. 12). Thus each crossing at $\tilde{k}_1^*$ comes with a partner at $-\tilde{k}_1^* - \pi$ and the total number of crossing in the half spectrum $\tilde{k}_1 \in (-\pi, 0)$ must be even. We can always avoid a crossing at the degenerate point $\tilde{k}_1^* = -\pi/2 = -\tilde{k}_1^* - \pi$ where this argument breaks down by changing $\tilde{\vartheta}^*$, since it is arbitrary.

Appendix E: $C_{2x}T$ symmetry

In this Appendix, we discuss the Hofstadter topological phases protected by $C_{2x}T$ symmetry. First, we demonstrate that $(UC_{2x}T)^2 = \pm(C_{2x}T)^2$ where the sign is determined by an integral along Peierls paths (App. E1). We discuss the topological invariants in both cases. If $(UC_{2x}T)^2 = +1$, the $w_2$ invariant at $\Phi/2$ can be calculated in an expanded unit cell where $U$ is diagonal in momentum space (App. E2). When $(UC_{2x}T)^2 = -1$, we argue the phase must be trivial in real space, and then calculate the nested Wilson loop to show the triviality explicitly (App. E3).

1. Symmetry Properties

In Sec. , we consider Hamiltonians with the symmetry $C_{2x}T$ at $\phi = 0$ which satisfies $(C_{2x}T)^2 = +1$. At $\phi = \Phi/2$, the symmetry of $H^{\phi/2}$ is $UC_{2x}T$, which may square to either $\pm 1$. We derive a formula for this sign as follows. First, the action of $C_{2x}$ on the annihilation operator reads

$$C^\dagger_{2x} c_{\bm{R},\alpha} C_{2x} = \sum_\beta D_{\alpha\beta}(C_{2x}) c_{-\bm{R} - \delta_\alpha - \delta_\beta, \beta}$$

(E1)

where $D_{\alpha\beta}(C_{2x}) = 0$ if $\delta_\alpha - C_{2x} \delta_\beta = \delta_\alpha + \delta_\beta$ is not a lattice vector. We let $U = e^{i\alpha}$ as defined by Eq. (A5), and then compute

$$C_{2x} O = C_{2x} \sum_{\bm{R},\beta} c^\dagger_{\bm{R},\beta} c_{\bm{R},\beta} \int_{r_0}^{R+\delta_\beta} \hat{\bm{A}} \cdot d\bm{r},$$

$$= \sum_{\bm{R},\beta} C_{2x} c^\dagger_{\bm{R},\beta} C_{2x} c_{\bm{R},\beta} C_{2x} \int_{r_0}^{R+\delta_\beta} \hat{\bm{A}} \cdot d\bm{r}$$

(E2)

$$= \left( \sum_{\beta, \beta', \beta''} c^\dagger_{\bm{R},\beta} - \delta_{\beta' \beta''} [D(C_{2x})^\dagger, D(C_{2x})]_{\beta' \beta''} c_{-\bm{R} - \delta_\beta - \delta_{\beta' \beta''}, \beta''} \int_{r_0}^{R+\delta_\beta} \hat{\bm{A}} \cdot d\bm{r} \right) C_{2x}$$

where $\nabla \times \hat{\bm{A}} = \Phi$ and the integral is taken along Peierls paths. Now we take $-\bm{R} - \delta_\beta - \delta_{\beta' \beta''} \rightarrow \bm{R}$ by relabeling the sum. This takes $c_{-\bm{R} - \delta_\beta - \delta_{\beta' \beta''}} \rightarrow c_{\bm{R} + \delta_{\beta' \beta''} - \delta_\beta, \beta''}$. But because $[D(C_{2x})^\dagger, D(C_{2x})]_{\beta' \beta''}$ is only nonzero when $\delta_{\beta' \beta''} = 0$ by unitarity, we have

$$C_{2x} O = \left( \sum_{\beta, \beta', \beta''} c^\dagger_{\bm{R},\beta} [D(C_{2x})^\dagger]_{\beta' \beta} [D(C_{2x})]_{\beta \beta''} c_{\bm{R},\beta''} \int_{r_0}^{R+\delta_\beta} \hat{\bm{A}} \cdot d\bm{r} \right) C_{2x}$$

(E3)
We recall for the reader that $\tilde{A}$ is a gauge field generating $\Phi$ flux. Hence, from Eq. (A4), we can deform the integral along Peierls paths to find

$$\int_{r_0}^{R - \delta_{\beta'}} \tilde{A} \cdot dr = \left( \int_{-r_0}^{R - \delta_{\beta'}} + \int_0^{r_0} \right) \tilde{A} \cdot dr \mod 2\pi . \tag{E4}$$

By a change of variables in the integral $r = -s$, we establish

$$\int_{-r_0}^{R - \delta_{\beta'}} \tilde{A}(r) \cdot dr = \int_{r_0}^{R + \delta_{\beta'}} \tilde{A}(-s) \cdot (-s) = \int_{r_0}^{R + \delta_{\beta'}} \tilde{A}(s) \cdot ds \tag{E5}$$

where we have used that $\tilde{A}(r)$ is an odd function of $r$. This allows us to write

$$C_{2z} O = \left( O + \left[ \int_{r_0}^{r_0} \tilde{A} \cdot dr \right] \sum_{R, \beta} c_R^\dagger c_{R, \beta} \right) C_{2z},$$

$$= \left( O + \left[ \int_{r_0}^{r_0} \tilde{A} \cdot dr \right] N \right) C_{2z}, \tag{E6}$$

where $N$ is the total number of electrons in the many-body state. In this work, we study single-particle physics where $N = 1$. In this case, we exponentiate Eq. (E6) to find

$$C_{2z} U = C_{2z} \sum_{n=0}^{\infty} \frac{1}{n!} (iO)^n \int_{r_0}^{r_0} \tilde{A} \cdot dr$$

$$= \sum_{n=0}^{\infty} \frac{1}{n!} \left[ O + \left[ \int_{r_0}^{r_0} \tilde{A} \cdot dr \right] \right]^n C_{2z}$$

$$= \exp \left( iO + i \left[ \int_{r_0}^{r_0} \tilde{A} \cdot dr \right] \right) C_{2z}$$

$$= \exp \left( i \int_{r_0}^{r_0} \tilde{A} \cdot dr \right) UC_{2z} \tag{E7}$$

where in the last line we use that $O$ commutes with the $c$-number $i \int_{r_0}^{r_0} \tilde{A} \cdot dr$. Using Eq. (E7) and the relation $TU = U^\dagger T$ (see Eq. (D3)), we find

$$(UC_{2z} T)^2 = UC_{2z} TUC_{2z} T$$

$$= UC_{2z} U^\dagger TC_{2z} T$$

$$= \exp \left( -i \int_{r_0}^{r_0} \tilde{A} \cdot dr \right) C_{2z} UU^\dagger TC_{2z} T$$

$$= \exp \left( -i \int_{r_0}^{r_0} \tilde{A} \cdot dr \right) C_{2z} TC_{2z} T$$

$$= \exp \left( -i \int_{r_0}^{r_0} \tilde{A} \cdot dr \right) \left( C_{2z} T \right)^2 . \tag{E8}$$

We recall that the integrals must be taken along the Peierls paths, and $r_0$ is a fixed but arbitrary orbital of the Hamiltonian (see Eq. (A5)). Additionally, in defining $C_{2z}$, we have fixed the origin of the lattice to coincide with the $C_{2z}$-symmetric point of $A$, i.e. $A(C_{2z} r) = -A(r)$. This fixes the origin of the lattice, so we cannot redefine $r_0$. Eq. (E8) demonstrates that $(UC_{2z} T)^2$ may differ from $(C_{2z} T)^2 = 1$ by a phase

$$\gamma_2 = \int_{r_0}^{r_0} \tilde{A} \cdot dr \mod 2\pi \tag{E9}$$

that depends only on the Peierls paths and orbitals of the Hamiltonian. It is simple to determine $\gamma_2$ by direct computation for a given model. But we show first that $\gamma_2$ may only take the value 0 or $\pi$, on the condition that the
Peierls paths of the model are themselves $C_{2z}$-symmetric. Let the path $\mathcal{C}_1$ consist of Peierls paths connecting $r_0$ to $C_2 r_0 = -r_0$, and define $\mathcal{C}_2 = C_{2z} \mathcal{C}_1$ which connects $-r_0$ to $r_0$. By the same change of variables, we have that

$$
\int_{\mathcal{C}_2} \mathbf{A} \cdot d\mathbf{r} = \int_{\mathcal{C}_2 + \mathcal{C}_1} \mathbf{A} \cdot d\mathbf{r} = \int_{\mathcal{C}_1} -\mathbf{A} \cdot d(-\mathbf{r}) = \int_{\mathcal{C}_1} \mathbf{A} \cdot d\mathbf{r} .
$$

(E10)

With this result, it is also true that

$$
\oint_{\mathcal{C}_1 + \mathcal{C}_2} \mathbf{A} \cdot d\mathbf{r} = \int_{\mathcal{C}_1} \mathbf{A} \cdot d\mathbf{r} + \int_{\mathcal{C}_2} \mathbf{A} \cdot d\mathbf{r} = 2 \int_{\mathcal{C}_1} \mathbf{A} \cdot d\mathbf{r} .
$$

(E11)

Because $\mathcal{C}_1$ and $\mathcal{C}_2$ are both Peierls paths, $\mathcal{C}_1 + \mathcal{C}_2 = \partial \mathcal{R}$ is a closed loop taken along Peierls paths, and thus

$$
2 \int_{r_0}^{-r_0} \mathbf{A} \cdot d\mathbf{r} = \oint_{\partial \mathcal{R}} \mathbf{A} \cdot d\mathbf{r} = \int_{\mathcal{R}} \Phi d\mathbf{S} \in 2\pi \mathbb{Z}
$$

(E12)

where we have used that $\nabla \times \mathbf{A} = \Phi$ and, by the definition of $\Phi$, all closed loops along Peierls’ paths enclose an integer multiple of 2$\pi$ flux. Hence find that $\int_{r_0}^{-r_0} \mathbf{A} \cdot d\mathbf{r}$ is a multiple of $\pi$ and thus the phase is quantized to be 0 or $\pi$.

The phase $\gamma_2$ may be calculated to determine the sign of $(UC_{2z}T)^2$. In some cases however, it may be determined more simply. For instance, if there is an orbital on the 1a = (0, 0) position, we may choose $r_0 = (0, 0)$ in which case the integration path vanishes and $\gamma_2$ must be zero. More generally, if there are any Peierls paths that connect $r_0$ to the origin, then we can break up the integral into $C_{2z}$-symmetric parts:

$$
\gamma_2 = \int_{r_0}^{-r_0} \mathbf{A} \cdot d\mathbf{r} = \int_{r_0}^{0} \mathbf{A} \cdot d\mathbf{r} + \int_{0}^{-r_0} \mathbf{A} \cdot d\mathbf{r} = -\int_{0}^{-r_0} \mathbf{A} \cdot d\mathbf{r} + \int_{0}^{r_0} \mathbf{A} \cdot d\mathbf{r} = -\int_{0}^{r_0} \mathbf{A} \cdot d\mathbf{r} + \int_{0}^{r_0} \mathbf{A} \cdot d\mathbf{r} = 0 .
$$

(E13)

We find that if the origin may be reached along Peierls path, then the phase is also forced to be zero. (We emphasize that at $\phi = \Phi$, integrals may be arbitrarily deformed along Peierls paths.) For the the QSH model of App. F1, orbitals lie on the 1a = (0, 0) position so the phase is trivial, and in the model of twisted bilayer graphene discussed in App. G1 the Peierls paths are taken through the origin as shown in Fig. 15a, so the phase must also be trivial. To furnish an example where the phase is $\pi$, we consider an alternative model of TBG in Ref. [37] that is identical to our model of TBG except for the choice of Peierls’ paths. In the alternative model, the Peierls paths are taken along the bonds, so that $\Phi = 2\pi$, as shown in Fig. 15b. We can calculate $\gamma_2$ directly via Eq. (E9). We choose $r_0 = \frac{1}{2} \mathbf{b}_1 - \frac{1}{2} \mathbf{a}_1$, the same as in Fig. 16 and calculate

$$
\gamma_2 = \int_{r_0}^{-r_0} \mathbf{A} \cdot d\mathbf{r} \mod 2\pi = \pi
$$

(E14)

where the path of integration (which is arbitrary as long as it is taken along Peierls paths) is shown in Fig. 15b. This emphasizes once more that the Peierls paths are physical. Different Peierls paths in the TBG model lead to different values of $\gamma_2$, giving $(UC_{2z}T)^2 = \pm (C_{2z}T)^2$. In general, $\gamma_2$ may be simply calculated from Eq. (E9) for any model. In coming work (Ref. [50]), we will show that similar phases $\gamma_n$ characterize the algebra of general $UC_n T$-symmetric point groups at high symmetry Wyckoff positions.

The sign of $(UC_{2z}T)^2$ has important physical consequences. If $(UC_{2z}T)^2 = +1$, then $UC_{2z}T$ protects a $w_2$ invariant at $\phi = \Phi/2$ in the same way as $C_{2z} T$ protects a $w_2$ invariant at $\phi = 0$. We discuss how to compute this invariant in App. E2 If $(UC_{2z}T)^2 = -1$, then there is no $w_2$ invariant [39]. In this case, we show in App. E3 using the nested Wilson and the 10 Fold Way that there is no nontrivial phase protected by $UC_{2z}T$, and hence $H^{\phi=\Phi/2}$ is trivial.

2. Calculation of the $w_2$ invariant at $(UC_{2z}T)^2 = +1$

In this section, we show how to use the Wilson loop to compute the $w_2$ index of $H^{\phi=\Phi/2}$. We work in the Landau gauge, which is best suited for explicit calculations. Recall from Ref. [39] that $w_2$ may be computed at $\phi = 0$ from the Wilson loop spectrum, which is “particle-hole” symmetric thanks to $C_{2z} T$ [8]. We can follow the same protocol at $\phi = \Phi/2$, but we will find that $U$ acts off-diagonally in momentum space and changes the symmetries of the Wilson spectrum.
FIG. 15. We show the Peierls paths joining \( r_0 \) and \(-r_0\) in (a) our model of twisted bilayer graphene and (b) an alternative model discussed in Ref. [37] where Peierls paths are taken along the bonds of the lattice. The different Peierls paths lead to different values of \( \gamma_2 \): +1 (resp. -1) in the case of our model (resp. the alternative model).

\[ a. \text{ Construction of the Extended unit cell} \]

To compute \( w_2 \) in the conventional way, we must construct \( U \) in an extended unit cell where it is diagonal in momentum space. We begin with the expression for \( U \) in a single-particle Hilbert space:

\[
U = \sum_{\mathbf{R}_0} \exp \left(i \int_{\mathbf{r}_0}^{\mathbf{R} + \mathbf{A}} \mathbf{A} \cdot d\mathbf{r} \right) |\mathbf{R}, \alpha\rangle \langle \mathbf{R}, \alpha|, \quad \mathbf{\nabla} \times \mathbf{A} = \Phi, \tag{E15}
\]

as is rewritten from Eq. [2] of the Main Text. Recall that the integral is taken along Peierls paths and is single-valued mod \( 2\pi \). Here we have used the single-particle bases \(|\mathbf{R}, \alpha\rangle\). To derive the action of \( U \) on the Hofstadter Hamiltonian \( H^{\phi=\Phi/2}(\mathbf{k}) \) in the Landau gauge, we could Fourier transform \( U \) over the 1 \( \times \) \( q' \) unit cell at \( \phi = \Phi/2 \), where \( \phi = \mu \frac{2\pi q'}{q} \) as discussed in App. A 7. (The gauge-independent formalism introduced in App. D 2 b which ensures \( H^{\phi=\Phi/2} \) periodicity does not generically share the \( 1 \times q' \) periodicity of \( H^{\phi=\Phi/2} \).) Hence, it has some minimal spatial periodicity \( (\lambda_1, \lambda_2) \) with \( \lambda_1, \lambda_2 \in \mathbb{N} \) given by

\[
\int_{\mathbf{r}_0}^{\lambda_1 \mathbf{a}_1 + \mathbf{R} + \mathbf{A}_0} \mathbf{A} \cdot d\mathbf{r} = \int_{\mathbf{r}_0}^{\lambda_2 \mathbf{a}_2 + \mathbf{R} + \mathbf{A}_0} \mathbf{A} \cdot d\mathbf{r} = \int_{\mathbf{r}_0}^{\mathbf{R} + \mathbf{A}_0} \mathbf{A} \cdot d\mathbf{r} \mod 2\pi, \quad \forall \alpha = 1, \ldots, N_{\text{orb}} \tag{E16}
\]

with \( \mathbf{R} \) being any lattice vector. (Although it is not necessary for any of the following calculations, we can show that \( \lambda_i \) is the denominator of \( \kappa_i \), defined in Eqs. [D30] and [D31], i.e. \( \lambda_i \kappa_i = 0 \mod 2\pi \). From this perspective, the magnetic unit cell is extended so translations by \( \lambda_i \mathbf{a}_i \) commute with \( U \mathcal{T} \), as we see from Eq. [D39].) When we Fourier transform over the Bravais lattice composed of the enlarged \( \lambda_1 \times \lambda_2 \) unit cells, the BZ shrinks to \( k_1 \in (-\frac{\pi}{\lambda_1}, \frac{\pi}{\lambda_1}) \), \( k_2 \in (-\frac{\pi}{\lambda_2}, \frac{\pi}{\lambda_2}) \) which we label as \( \text{BZ}_\lambda \). In this unit cell, the position bases are defined

\[
|\mathbf{r}_1, \mathbf{r}_2, \ell_1, \ell_2, \alpha\rangle = c_{(\ell_1 \mathbf{r}_1 + \ell_2 \mathbf{r}_2) \mathbf{a}_0} |0\rangle, \quad \ell_1 = 0, \ldots, \lambda_1 - 1, \quad \ell_2 = 0, \ldots, \lambda_2 - 1. \tag{E17}
\]

The momentum eigenstates are then defined by

\[
|\mathbf{r}_1, \mathbf{r}_2, \ell_1, \ell_2, \alpha\rangle = \frac{1}{\sqrt{N/\lambda_1 \lambda_2}} \sum_{k_1, k_2 \in \text{BZ}_\lambda} e^{i(k_1 \mathbf{b}_1 + k_2 \mathbf{b}_2):((\ell_1 \mathbf{r}_1 + \ell_2 \mathbf{r}_2) \mathbf{a}_1 + (\lambda_1 \mathbf{r}_1 + \ell_2 \mathbf{r}_2) \mathbf{a}_2 + \mathbf{A}_0)} |k_1, k_2, \ell_1, \ell_2, \alpha\rangle, \tag{E18}
\]
where \( N \) is the number of 1 \( \times \) 1 unit cells in the lattice. We may now compute

\[
U = \sum_{r_1, r_2, \ell_1, \ell_2, \alpha} \exp \left( i \int_{r_0}^{(\lambda_1 r_1 + \ell_1) a_1 + (\lambda_2 r_2 + \ell_2) a_2 + \delta_\alpha} \tilde{A} \cdot dr \right) |r_1, r_2, \ell_1, \ell_2, \alpha\rangle \langle r_1, r_2, \ell_1, \ell_2, \alpha|
\]

\[
= \frac{1}{N/\lambda_1 \lambda_2} \sum_{\mathbf{k}, \mathbf{k}' \in BZ, \ell_1, \ell_2, \alpha} |\mathbf{k}, \ell_1, \ell_2, \alpha\rangle \langle \mathbf{k}', \ell_1, \ell_2, \alpha| \times
\left[ \sum_{r_1, r_2} \exp \left( i (\mathbf{k} - \mathbf{k}') \cdot ((\lambda_1 r_1 + \ell_1) a_1 + (\lambda_2 r_2 + \ell_2) a_2 + \delta_\alpha) \right) \right] \exp \left( i \int_{r_0}^{(\lambda_1 r_1 + \ell_1) a_1 + (\lambda_2 r_2 + \ell_2) a_2 + \delta_\alpha} \tilde{A} \cdot dr \right)
\]

\[
= \frac{1}{N/\lambda_1 \lambda_2} \sum_{\mathbf{k}, \mathbf{k}' \in BZ, \ell_1, \ell_2, \alpha} |\mathbf{k}, \ell_1, \ell_2, \alpha\rangle \langle \mathbf{k}', \ell_1, \ell_2, \alpha| \times
\left[ \sum_{r_1, r_2} \exp \left( i (\mathbf{k} - \mathbf{k}') \cdot ((\lambda_1 r_1 + \ell_1) a_1 + (\lambda_2 r_2 + \ell_2) a_2 + \delta_\alpha) \right) \right] \exp \left( i \int_{r_0}^{\ell_1 a_1 + \ell_2 a_2 + \delta_\alpha} \tilde{A} \cdot dr \right)
\]

(E19)

where we have used Eq. (E16) to remove the \( r_1, r_2 \) dependence of the integral. Then the sum in brackets can be explicitly evaluated and we find

\[
U = \frac{1}{N/\lambda_1 \lambda_2} \sum_{\mathbf{k}, \mathbf{k}' \in BZ, \ell_1, \ell_2, \alpha} |\mathbf{k}, \ell_1, \ell_2, \alpha\rangle \langle \mathbf{k}', \ell_1, \ell_2, \alpha| e^{i \int_{r_0}^{\ell_1 a_1 + \ell_2 a_2 + \delta_\alpha} \tilde{A} \cdot dr + i (\mathbf{k} - \mathbf{k}') \cdot (\ell_1 a_1 + \ell_2 a_2 + \delta_\alpha)} \times
\left[ \sum_{r_1, r_2} e^{i (\mathbf{k} - \mathbf{k}') \cdot (\lambda_1 r_1 a_1 + \lambda_2 r_2 a_2)} \right]
\]

(E20)

We see explicitly that \( U \) is diagonal in momentum space in the \( \lambda_1 \times \lambda_2 \) unit cell.

We now give an example of this calculation for model of twisted bilayer graphene (introduced in detail in App. G1). In fact, we will use this expression for \( U \) in momentum space later for Wilson loop calculations in App. G3. We recall that the nearest-neighbor vectors of the honeycomb lattice are \( \delta_\alpha, \alpha = 1, 2, 3 \) (as shown for convenience in Fig. 16), and that there are \( s \) and \( p_z \) orbitals on the atomic sites which are located at \( \pm \frac{1}{2} \delta_1 - \frac{1}{2} a_1 \). We refer to the choice of + (resp. −) as the (resp. B) sublattice. The Peierls paths of the model (Fig. 3) enclosed multiples of a third of the unit cell, so \( n = 3 \) and \( \Phi = 6 \pi \). Using our Landau gauge for \( \tilde{A} \), it is straightforward to calculate the following integrals along Peierls’ paths (see Fig. 3)

\[
\exp \left( i \int_{\mathbf{R} + \delta_\alpha}^{\mathbf{R} + \delta_\alpha \pm a_1} \tilde{A} \cdot dr \right) = -1, \quad \exp \left( i \int_{\frac{1}{2} \delta_1 - \frac{1}{2} a_1}^{\frac{1}{2} \delta_1 - \frac{1}{2} a_1} \tilde{A} \cdot dr \right) = -1.
\]

(E21)
where we have used Eq. (E20) to determine the action of $U$ which we show pictorially in Fig. 16b. According to Eq. (E16), we can choose a 2
\[
\phi
\]
Hamiltonian at $BZ$ for brevity, we let
\[
\invariant \text{ and is not affected by the choice of unit cell. This is in contrast to the relative winding of the Wilson loop}
\]
\[
\vartheta
\]
\[
H
\]
\[
U
\]
\[
\text{sublattice. We will use this result in App. G3.}
\]
\[
\text{To begin, we can construct the extended unit cell to be}
\]
\[
\text{We define the}
\]
\[
\text{invariant to be calculated by counting the number of points where $\vartheta(\mathbf{k}) = 0$ and $\vartheta(\mathbf{k}) = \pi$ as described in Ref. [30]. We emphasize that $w_2^{\Phi/2}$ is a topological invariant and is not affected by the choice of unit cell. This is in contrast to the relative winding of the Wilson loop eigenvalues which may change when the unit cell is expanded.}
\]
\[
\text{To begin, we can construct the extended unit cell to be}
\]
\[
\lambda_1 \times \lambda_2 q'/gcd(\lambda_2, q')
\]
\[
H_{\Phi/2}^{\Phi/2}
\]
\[
\text{We define the 4th energy eigenstate of $H_{\Phi/2}^{\Phi/2}$ as $|u_{\Phi/2}^{\Phi/2}\rangle$ which is an $N_{orh} \times \lambda_1 \lambda_2$ vector. We call the representation of $UC_{2z} \mathcal{T}$ on the $|u_{\Phi/2}^{\Phi/2}\rangle$ eigenstates $D[UC_{2z} \mathcal{T}] = QK$ for brevity. We can derive an explicit expression by acting $UC_{2z} \mathcal{T}$ on the momentum eigenstates:}
\[
UC_{2z} \mathcal{T} |\mathbf{k}, \ell_1, \ell_2, \alpha\rangle = UC_{2z} \mathcal{T} \frac{1}{\sqrt{\lambda_1 \lambda_2}} \sum_{r_1, r_2} e^{-i\mathbf{k} \cdot \mathbf{r}_0} |(\lambda_1 \ell_1 + \ell_1) \mathbf{a}_1 + (\lambda_2 \ell_2 + \ell_2) \mathbf{a}_2 + \mathbf{d}_\alpha\rangle |r_1, r_2, \ell_1, \ell_2, \alpha\rangle
\]
\[
= \frac{1}{\sqrt{\lambda_1 \lambda_2}} \sum_{r_1, r_2} e^{-i(-\mathbf{k}) \cdot (\lambda_1 \ell_1 + \ell_1) \mathbf{a}_1 + (\lambda_2 \ell_2 + \ell_2) \mathbf{a}_2 + \mathbf{d}_\alpha} UC_{2z} \mathcal{T} |r_1, r_2, \ell_1, \ell_2, \alpha\rangle
\]
\[
= \frac{1}{\sqrt{\lambda_1 \lambda_2}} \sum_{r_1, r_2, \beta} e^{-i(-\mathbf{k}) \cdot (\lambda_1 \ell_1 + \ell_1) \mathbf{a}_1 + (\lambda_2 \ell_2 + \ell_2) \mathbf{a}_2 + \mathbf{d}_\alpha} UC_{2z} \mathcal{T} |r_1, r_2, \ell_1, \ell_2, \alpha\rangle
\]
\[
= \sum_{\beta} UC_{2z} \mathcal{T} |r_1, r_2, \ell_1, \ell_2, \alpha\rangle
\]
\[
\text{where we have used Eq. (E20) to determine the action of $U$ on the states. Now we define}
\]
\[
\mathcal{Q}_{\ell_1, \ell_2, \alpha, \ell_1', \ell_2', \beta} = UC_{2z} \mathcal{T} D[\mathcal{C}_{2z} \mathcal{T}]_{\alpha\beta} |r_1, r_2, -\ell_1, -\ell_2, \beta\rangle
\]
\[
\text{(E25)}
\]
\[
\text{(E26)}
\]
Note from Eq. \([E25]\) that \(Q_{\ell_1 \ell_2 \alpha, \ell'_1 \ell'_2 \beta}\) is only nonzero when \(\ell_1 a_1 + \ell_2 a_2 + \delta_\alpha = -(\ell'_1 a_1 + \ell'_2 a_2 + \delta_\beta) \mod \lambda_1 a_1 + \lambda'_2 a_2\). This is the usual constraint on spatial symmetries, but in the expanded unit cell. Using this property, we can expand from Eq. \([E25]\) to find

\[
UC_{2z} T |k, \ell_1, \ell_2, \alpha\rangle = \frac{1}{\sqrt{N/\lambda_1 \lambda'} \sum_{r_1, r_2, \ell'_1, \ell'_2, \alpha}} e^{-i(k - (\lambda_1 r_1 + \ell'_1) a_1 + (\lambda'_2 r_2 + \ell'_2) a_2 - \delta_\beta)} [Q]_{\ell_1 \ell_2 \alpha, \ell'_1 \ell'_2 \beta} |r_1, r_2, \ell', \ell', \beta\rangle K
\]

\[
= \frac{1}{\sqrt{N/\lambda_1 \lambda'} \sum_{r_1, r_2, \ell'_1, \ell'_2, \alpha}} e^{-ik - (\lambda_1 r_1 + \ell'_1) a_1 + (\lambda'_2 r_2 + \ell'_2) a_2 - \delta_\beta} [Q]_{\ell_1 \ell_2 \alpha, \ell'_1 \ell'_2 \beta} |r_1, r_2, \ell', \ell', \beta\rangle K
\]

\[
= \sum_{\ell'_1, \ell'_2, \alpha} [Q]_{\ell_1 \ell_2 \alpha, \ell'_1 \ell'_2 \beta} |k, \ell'_1, \ell'_2, \beta\rangle K^\dagger.
\]

We assume that \((UC_{2z} T)^2 = +1\) in this section, so \(QQ^* = +1\). Note that in the \(\lambda_1 \times \lambda'_2\) unit cell, \(UC_{2z} T\) is also diagonal in momentum space because both \(C_{2z}\) and \(T\) reverse the momentum of a state. Then we can define a unitary sewing matrix

\[
B_{k}^{ij} = \langle u_i^{\Phi/2}(k)|Q|u_j^{\Phi/2*}(k)\rangle
\]

which obeys

\[
|u_j^{\Phi/2}(k)\rangle = Q |u_i^{\Phi/2*}(k)\rangle [B^\dagger]_{k}^{ij}.
\]

Using Eq. \([E29]\), we determine that a small segment of a Wilson loop obeys

\[
[W_{k_1 \rightarrow k_1}^{\Phi/2}]_{ij} = \langle u_i^{\Phi/2}(k_1)| u_j^{\Phi/2}(k_1)\rangle
\]

\[
= \sum_{r,s} B_{k_1}^{rs} \langle u_i^{\Phi/2*}(k_1)|Q|u_s^{\Phi/2*}(k_1)\rangle [B^\dagger]_{k_1}^{sj}
\]

\[
= \sum_{r,s} B_{k_1}^{rs} [W_{k_1 \rightarrow k_1}^{\Phi/2*}]_{rs} [B^\dagger]_{k_1}^{sj}.
\]

Extending this to a full Wilson loop along \(BZ_{\lambda'}\), where we integrate along \(k_2 \in (0, 2\pi/\lambda'_2)\), we find

\[
W^{\Phi/2}(k_1) = B(k_1, \frac{2\pi}{\lambda'_2}) W^{\Phi/2*}((k_1, \frac{2\pi}{\lambda'_2}) B^\dagger(k_1, 0)
\]

\[
= B(k_1, \frac{2\pi}{\lambda'_2}) W^{\Phi/2*}(k_1) B^\dagger(k_1, 0)
\]

To related the sewing matrices \(B\) at points across the \(BZ_{\lambda'}\), we need to use the embedding matrix \(V_2' (\Phi/2)\) that implements the \(2\pi/\lambda'_2\) periodicity. Following identically the calculation of the the embedding matrix \(V_2 (\phi)\) in the \(1 \times q'\) unit cell in Eq. \([A44]\), we find

\[
[V_2' (\Phi/2)]_{\ell_1 \ell_2 \alpha, \ell'_1 \ell'_2 \beta} = \delta_{\ell_1 \ell'_1} \delta_{\ell_2 \ell'_2} e^{i \frac{2\pi}{\lambda'_2} \ell_2 \alpha} e^{i \frac{2\pi}{\lambda'_2} \ell_2 \beta}
\]

where \(\ell_1 = 0, \ldots, \lambda_1 - 1\) and \(\ell_2 = 0, \ldots, \lambda'_2 - 1\) index the unit cells within the extended \(\lambda_1 \times \lambda'_2\) unit cell, respectively. We now observe that

\[
B(k_1, \frac{2\pi}{\lambda'_2}) = \langle u_i^{\Phi/2}(k_1, \frac{2\pi}{\lambda'_2})|QK|u_j^{\Phi/2}(k_1, \frac{2\pi}{\lambda'_2})\rangle
\]

\[
= \langle u_i^{\Phi/2}(k_1, 0)|QK|u_j^{\Phi/2}(k_1, 0)\rangle
\]

By direct calculation with Eqs. \([E26]\) and \([E32]\), we compute

\[
[V_2' (\Phi/2)] W K V_2' (\Phi/2)]_{\ell_1 \ell_2 \alpha, \ell'_1 \ell'_2 \beta} = e^{-i \frac{2\pi}{\lambda'_2} (\ell_2 a_2 + \delta a_2 + \ell_2 a_2 + \delta \beta) \cdot b_2} [QK]_{\ell_1 \ell_2 \alpha, \ell'_1 \ell'_2 \beta}
\]

\[
= [QK]_{\ell_1 \ell_2 \alpha, \ell'_1 \ell'_2 \beta}
\]

where in the last line we have used that \([QK]_{\ell_1 \ell_2 \alpha, \ell'_1 \ell'_2 \beta}\) is only nonzero if \(\ell_1 a_1 + \ell_2 a_2 + \delta \alpha = -(\ell'_1 a_1 + \ell'_2 a_2 + \delta \beta) \mod \lambda_1 a_1 + \lambda'_2 a_2\), so \(\ell_2 + \delta \alpha \cdot b_2 + \ell'_2 + \delta \beta \cdot b_2 = 0 \mod \lambda'_2\). Hence we obtain

\[
B_{k}^{ij} = \langle u_i^{\Phi/2}(k_1, 0)|QK|u_j^{\Phi/2}(k_1, 0)\rangle
\]

\[
= B_{k}^{ij}.
\]

\[
(E35)
\]
Returning to Eq. (E31), we find the desired “particle-hole” symmetry

\[
W^{\Phi/2}(k_1) = B^\dagger(k_{1,0}) W^{\Phi/2 \ast}(k_1) B(k_{1,0}),
\]
\[
\{ \partial_j(k_1) \} = \{-\partial_j(k_1) \}
\]  \hspace{1cm} \text{(E36)}

as previously stated. This is identical to the Wannier center constraint arising from \(C_{2z}T\) at \(\phi = 0\) and hence we can calculate \(w_2\) directly from the Wilson loop spectrum following the discussion of Ref. [30].

3. Proof of a Trivial Phase when \((UC_{2z}T)^2 = -1\)

Now we consider the case where \((UC_{2z}T)^2 = -1\) and there is no \(w_2\) invariant defined. We remark that no 2D crystalline system at \(\phi = 0\) can have such a symmetry because \((C_{2z}T)^2 = C_{2z}^2 T^2 = (\pm 1)^2 = 1\). From the 3D perspective where \(\phi\) is interpreted as \(k_z\) and \(U\) is the embedding matrix along the \(z\) direction, the symmetry algebra at \(k_z = 0\) is always the same as at \(k_z = \pi\), so having \((C_{2z}T)^2 = +1\) and \((UC_{2z}T)^2 = -1\) is also impossible. The possibility of such projective symmetry algebras (see also Eq. (D39)) is a novel feature of Hofstadter physics.

The Higher Order Topological Insulator (HOTI) phase is still characterized by Wannier flow between \(w_\mu\) for \(\mu = 0\) in the bulk. Because we assume a non-trivial \(w_2\) index at \(\phi = 0\) that protects corner states, we need only show corner states are not stable if \((UC_{2z}T)^2 = -1\). This establishes that \(H^{\Phi/2}\) is in a trivial atomic limit, and so pumping must occur between \(\phi = \Phi/2\) and \(\phi = 0\).

First we provide a heuristic argument that \((UC_{2z}T)^2 = -1\) trivializes the phase. First we consider the boundary signatures. We consider a high symmetry Wyckoff position \(w\) with \(UC_{2z}T\) in its magnetic point group. If the state has a center exactly at \(w\), then by Kramers Theorem it must have a Kramers partner at \(w\). If a state has a Wannier center at \(w + \delta\), perturbed slightly from \(w\), then by \(UC_{2z}T\) there is another state at \(w - \delta\). Hence any pair of states at \(w\) can be moved adiabatically away from \(w\) along \(UC_{2z}T\)-symmetric paths. This indicates a trivial RSI [51]. In coming work (Ref. [54]), we derive expressions for the RISIs of all the 2D magnetic point groups.

In absence of the \(w_2\) invariant, corner states can still be diagnosed using the nested Berry phase formalism of Refs. [35, 50]. Hence, we can compute the determinant of the nested Wilson loop \(W\) to confirm the heuristic argument given before. We remark that Ref. [57] demonstrated that \(C_{2z}T\) symmetry quantizes \(\text{det} W = \pm 1\) (where \(-1\) is the nontrivial value of the topological phase) when \((C_{2z}T)^2 = \pm 1\) and the nested Wilson loop is taken over a particle-hole symmetric configuration of Wannier bands. Here we study the specific case where \((UC_{2z}T)^2 = -1\), and we show that the determinant of the nested Wilson loop over particle-hole symmetric Wannier bands is fixed to be +1, trivial.

We define the Wannier Hamiltonian \(H_W(k_1)\) by \(W^{\Phi/2}(k_1) = e^{iH_W(k_1)}\), and the Wannier bands as

\[
H_W(k_1) |w_j(k_1)\rangle = \partial_j(k_1) |w_j(k_1)\rangle.
\]  \hspace{1cm} \text{(E37)}

We call \(\mathcal{K} = B(k_{1,0})K\) the representation of \(UC_{2z}T\) on \(H_W(k_1)\) such that

\[
\mathcal{K} H_W(k_1) \mathcal{K}^{-1} = -H_W(k_1).
\]  \hspace{1cm} \text{(E38)}

The essential difference between the \(\mathcal{K}^2 = +1\) case and the \(\mathcal{K}^2 = -1\) case is that the latter creates “anti-Kramers’ pairs”, i.e. the states \(|w_j(k_1)\rangle\) and \(\mathcal{K} |w_j(k_1)\rangle\) have opposite Wilson eigenvalues, \(\pm \partial(k_1)\), but are necessarily distinct even when \(\partial(k_1) = -\partial(k_1)\mod 2\pi\). First we prove that the two states \(|w(k_1)\rangle\) and \(\mathcal{K} |w(k_1)\rangle\) have opposite eigenvalues. Let \(H_W(k_1) |w(k_1)\rangle = \partial(k_1) |w(k_1)\rangle\). Then

\[
H_W(k_1) \mathcal{K} |w(k_1)\rangle = -\mathcal{K} H_W(k_1) |w(k_1)\rangle
= -\mathcal{K} \partial(k_1) |w(k_1)\rangle
= -\partial(k_1) \mathcal{K} |w(k_1)\rangle
\]  \hspace{1cm} \text{(E39)}

where we have used Eq. (E38) to anti-commute \(\mathcal{K}\) and \(H_W(k_1)\). Now we prove that anti-Kramers’ pairs represent distinct states by contradiction. Suppose \(\partial(k_1) = 0, \pi\) and \(\mathcal{K}^{-1} |w_j(k_1)\rangle\) and \(|w_j(k_1)\rangle\) represent the same state, so
$\mathcal{K} |w_j(k_1)\rangle = e^{i\alpha} |w_j(k_1)\rangle$. Then by acting $\mathcal{K}$ again, we find

$$
\begin{align*}
\mathcal{K}^2 |w_j(k_1)\rangle &= \mathcal{K} e^{i\alpha} |w_j(k_1)\rangle \\
&= |w_j(k_1)\rangle + e^{-i\alpha}\mathcal{K} |w_j(k_1)\rangle \\
&= |w_j(k_1)\rangle + e^{-i\alpha} |w_j(k_1)\rangle \\
&= |w_j(k_1)\rangle.
\end{align*}
$$

so we reach a contradiction because $|w_j(k_1)\rangle \neq 0$. Importantly, we see that for $\vartheta = 0$ or $\vartheta = \pi$, where $\vartheta = -\vartheta$, $|w(k_1)\rangle$ and $\mathcal{K} |w(k_1)\rangle$ are true Kramers’ partners, meaning they are distinct states with the same eigenvalue.

Following Ref. [57], the Wilson loop bands selected to compute the nested Wilson loop should preserve $UC_2 T$. By Eq. (E39), the states $|w(k_1)\rangle$ and $\mathcal{K} |w(k_1)\rangle$ are automatically particle-hole symmetric and hence respect $UC_2 T$. We now argue that the bands of a generic nested Wilson loop can be gapped into pairs related by $\mathcal{K}$ because there are no other unitary symmetries to protect crossings, so in general the selected bands decompose into two sets, one above $\vartheta = 0$ and the other below $\vartheta = 0$. Note that there must always be an even number of bands because $(UC_2 T)^2 = -1$.

For now, we assume that there at least 4 bands so we can calculate the nested Wilson loop on a $UC_2 T$-symmetric pair of bands which is a subset of full Wilson Hamiltonian spectrum. We treat the special case of two bands later and show it is also trivial.

We now study a generic $2 \times 2$ block to show that its determinant is always +1, which is sufficient to establish that the determinant of a generic nested Wilson loop (with at least four bands) is +1 by block diagonalization. At every $k_1$, we can diagonalize the Wilson Hamiltonian $H_W(k_1)$ to find its two eigenvectors which, due to the $UC_2 T$ symmetry, can be written as $|w(k_1)\rangle$ and $\mathcal{K} |w(k_1)\rangle$. The nested Wilson loop in the $k_1 \in (-\pi/\lambda_1, \pi/\lambda_1), k_2 \in (0, 2\pi/\lambda_2)^x$ BZ of the extended unit cell is written

$$
\mathcal{W} = \tilde{U}^{\dagger}(2\pi/\lambda_1) \begin{bmatrix} 2\pi/\lambda_1 i\sigma & 0 \\ \Pi_{k_1} \end{bmatrix} \hat{U}(0), \quad \hat{P}_{k_1} = \tilde{U}(k_1)\tilde{U}^{\dagger}(k_1)
$$

where $\tilde{U}(k_1)$ is the $\lambda_1 \lambda_2^x N_{\text{orb}} \times 2$ matrix of the eigenvectors of the Wilson loop. We choose a conventional ordering where the columns of $U(k_1)$ are ordered such that $\tilde{U}(k_1) = [w_1(k_1), w_2(k_1)]$ where $w_1(k_1)$ is the column vector of length $\lambda_1 \lambda_2^x N_{\text{orb}}$ corresponding to $|w(k_1)\rangle$ and $w_2(k_1)$ is the column vector corresponding to $\mathcal{K} |w(k_1)\rangle$. Note that in this ordering,

$$
\begin{align*}
\mathcal{K} \tilde{U}(k_1) &= \mathcal{K} [w_1(k_1), w_2(k_1)] \\
&= [\mathcal{K} w_1(k_1), \mathcal{K} w_2(k_1)] K \\
&= [w_2(k_1), \mathcal{K}^2 w_1(k_1)] K \\
&= [w_2(k_1), -w_1(k_1)] K \\
&= [w_1(k_1), w_2(k_1)] \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} K \\
&= \tilde{U}(k_1) (-i\sigma_2 K)
\end{align*}
$$

where $\sigma_2$ is a Pauli matrix. Acting on the projectors, we find that they commute with $\mathcal{K}$:

$$
\begin{align*}
\mathcal{K} \hat{P}_{k_1} &= \tilde{U}(k_1) (-i\sigma_2 K) U^{\dagger}(k_1) \\
&= \tilde{U}(k_1) U^{\dagger}(k_1) (-i\sigma_2 K) \\
&= \tilde{U}(k_1) (-i\sigma_2 K) \\
&= -\tilde{U}(k_1) U^{\dagger}(k_1) K^{-1} \\
&= \tilde{U}(k_1) U^{\dagger}(k_1) K \\
&= \hat{P}_{k_1} K.
\end{align*}
$$

so $[\hat{P}_{k_1}, \mathcal{K}] = 0$. Using this identity on the nested Wilson loop, we find $(-i\sigma_2 K) \mathcal{W} (-i\sigma_2 K)^{\dagger} = \mathcal{W}$. Writing

$$
\mathcal{W} = e^{i\mathcal{H}_W}, \quad \mathcal{H}_W = \sum_{i=0}^{3} d_i \sigma_i,
$$
defining $\sigma_0$ as the $2 \times 2$ identity matrix, we find that $\mathcal{H}_W$ must obey

$$-\sigma_2 \mathcal{H}_W^* \sigma_2 = \mathcal{H}_W .$$

(E45)

Eq. (E45) requires $d_0 = 0$ or $d_0 = \pi$, but the $d_i$ for $i = 1, 2, 3$, are free. We emphasize that the anti-symmetric $\sigma_2$ matrix appearing in Eq. (E45) is due to $K^2 = -1$. In the other case where $K^2 = +1$, we could choose a symmetric matrix, like $\sigma_1$, and we would have a different reality condition. We can now compute the determinant from Eq. (E44):

$$\det(W) = \exp(i \text{Tr} [\mathcal{H}_W]) = \exp(2i d_0),$$

(E46)

so because $d_0$ is quantized by $UC_{2z} \mathcal{T}$ to be 0 or $\pi$, the determinant must equal $+1$. Thus for a Wilson loop with four or more bands, the nested Wilson loop indicates a trivial phase.

We now consider the special case of a Wilson loop $W^{\Phi/2}(k_1) = e^{iH_W(k_1)}$ with only two bands, so it is not possible to take a $UC_{2z} \mathcal{T}$-symmetric subset of bands. The $2 \times 2$ Wilson Hamiltonian $H_W(k_1)$ obeys $KH_W(k_1)K^{-1} = -H_W(k_1)$ with $K^2 = -1$. Without loss of generality, we make take $K = i\sigma_2 K$. We can apply the same reasoning of Eqs. (E44) and (E45) but for the Wilson Hamiltonian. We have that $H_W(k_1)$ must be in the form

$$H_W(k_1) = \sum_{i=0}^{3} h_{W,i}(k_1) \sigma_i$$

(E47)

where $h_{W,0}(k_1) = 0$ or $h_{W,0}(k_1) = \pi$ but $h_{W,i}(k_1)$ for $i = 1, 2, 3$ are free. Because the $h_{W,i}$ are free, there are no protected crossings (Weyl nodes) at $\vartheta = 0$ or $\vartheta = \pi$ and no protected winding number, unlike in the $(C_{2z} \mathcal{T})^2 = +1$ case studied in Ref. [8]. Indeed, the Wilson Hamiltonian Eq. (E47) must be topologically trivial as a map from $k_1 \in S^3$ to $h_{W,i} \in S^3$ because $\tau_1(S^3) = 0$. Thus we have shown that with $UC_{2z} \mathcal{T}$ symmetry satisfying $(UC_{2z} \mathcal{T})^2 = -1$, the Wilson loop with two bands is topologically trivial.

There is also a more abstract way to understand that $(UC_{2z} \mathcal{T})^2 = -1$ ensures the Wilson Hamiltonian is trivial. Returning to Eq. (E38), we recognize that the Wilson Hamiltonian (assuming $K^2 = -1$ is the only symmetry of the model) is in the symmetry class $C, d = 1$ of the Ten-fold Way [58, 59]. Therefore it has no topological index and is necessarily trivial. In comparison, when we consider $UC_{2z} \mathcal{T}$ symmetry squaring to $+1$, the Wilson Hamiltonian would be in the symmetry class $D, d = 1$ in which case there is a $\mathbb{Z}_2$ topological invariant which we identify as the quantized determinant of the nested Wilson loop [8, 57].

Appendix F: The Quantum Spin Hall Model

In this Appendix, we introduce the Quantum Spin Hall (QSH) model of Bernevig, Hughes, and Zhang (BHZ) as a simple lattice model to exemplify our proofs of the Hofstadter topological phase in Secs. and [24]. In App. F 1, we recap the essentials of the model before explicitly writing down the Hofstadter Hamiltonian. We enumerate the symmetries of the model and introduce onsite symmetry-breaking perturbations that isolate different topological phases: a mirror Chern insulator, a Kane-Mele insulator, and a fragile $w_3$ insulator. We then add a next-nearest neighbor term to the Hamiltonian to break the flux periodicity from $\Phi = 2\pi$ ($n = 1$) to $\Phi = 4\pi$ ($n = 2$). Using this model, we demonstrate that when $n$ is even, the Hofstadter phase of a zero-field $\mathbb{Z}_2$ insulator may be a weak TI or 3D (strong) TI (App. F 2).

1. Hofstadter Hamiltonian

The BHZ Hamiltonian is a model with spin-1/2 electrons $\sigma$ and $s, p$ orbitals $\tau$, all at the 1a Wyckoff position [24]. The momentum space Hamiltonian is

$$H_{QSH}(k_x, k_y) = (M - \cos k_x - \cos k_y)I \otimes \tau_3 + \sin k_x \sigma_3 \otimes \tau_1 + \sin k_y I \otimes \tau_2$$

(F1)

and realizes a Quantum Spin Hall effect with a mirror Chern number equal to $-1$ (resp. $+1$) for $0 < M < 2$ (resp. $-2 < M < 0$). We define this topological invariant using the mirror symmetry $M_z = -i\sigma_3 \otimes I$, the product of a rotation $C_{2z} = -i\sigma_3 \otimes \tau_3$ and inversion $I = I \otimes \tau_3$ which satisfies $[H_{QSH}(k), M_z] = 0$ for any $k$. Because $M_z$ is local in the BZ, all occupied bands can be labeled by a mirror eigenvalue $m = \pm i$. Then we define the usual Chern number $C$ and mirror Chern number $C_{M_z}$

$$C = C_{m=+i} + C_{m=-i}, \quad C_{M_z} = \frac{C_{m=+i} - C_{m=-i}}{2}$$

(F2)
use the C Ref. [50], we will develop the full theory of space group symmetries in the Hofstadter Butterfly. Because we do not

D by a permutation matrix

D the Hofstadter Hamiltonian is

µ

because

2

neighbor. The Peierls paths are taken along the lattice vectors, indicated by

C

1

FIG. 17. (a) We show the Peierls paths for the QSH model of App. F 1 with the hopping amplitudes. All orbitals are on the

1a Wyckoff position and, being s (blue) and p, (red) orbitals, are localized near the atoms. and the only hoppings are nearest

neighbor. (b) We show the lattice with the vector field A = φ(−y, 0) and the two hoppings in an arbitrary unit cell. We see that along C1, there is a nonzero phase accumulated along the hopping, but there is no phase accumulated along C2 because A is always perpendicular to the path of integration.

From these expressions, one can calculate that at half filling, the Chern number C is identically zero (owing to TRS) but that

\[ C_M = \begin{cases} -1, & M \in (0, 2) \\ +1, & M \in (-2, 0) \\ 0, & |M| > 2 \end{cases} \] (F3)

As per the discussion in Sec., the Hofstadter Butterfly must have a gap closing when |M| < 2 since each mirror block of the Hamiltonian has its own non-zero Chern number. To verify this, we construct the Hofstadter Hamiltonian explicitly.

The Hofstadter Hamiltonian is simple to construct because all hoppings are nearest neighbor and we take the Peierls path directly along the bonds for all orbitals in the model, as shown in Fig. 17a. In our Landau gauge A = (−φy, 0), the only term that acquires a phase the y-hopping: \( c_{x+1,y}^\dagger c_{x,y} \rightarrow e^{-i\phi y}c_{x+1,y}^\dagger c_{x,y} \) as we depict Fig. 17b. All closed loops enclose an integer area, so \( n = 1 \), and we can take \( \phi = \frac{2\pi n}{q} \) to recover a \( 1 \times q \) magnetic unit cell. (Note that because \( \mu = 1 \), there is no distinction between \( q \) and \( q' \) in this gauge.) At \( \Phi = 2\pi \), all the Peierls phases of the model are manifestly zero mod \( 2\pi \), so it can be trivially shown that the \( H^{\phi+\Phi} = H^\phi \), and hence \( U = 1 \) (Eq. (A5)). The Hofstadter Hamiltonian is

\[ H_{y,y'}^{\phi} = \delta_{y,y'}h_y + \delta_{y,y'+1}T + \delta_{y+1,y'}T^\dagger \\
\ h_y = (M - \cos(k_x - \phi y))I \otimes \tau_3 + \sin(k_x - \phi y)\sigma_3 \otimes \tau_1, \] (F4)

\[ T = -\frac{1}{2} e^{-i\pi y} I \otimes (\tau_3 - i\tau_2) \]

We promote the Mirror symmetry to \( M_z = \delta_{y,y'}(-i\sigma_3 \otimes I) \) since it commutes with each block of the Hofstadter Hamiltonian. Thus we see explicitly that \( M_z \) remains a symmetry at all \( \phi \).

As discussed in Sec., we add symmetry-breaking terms to the QSH model Eq. (17) to remove symmetries from the Hamiltonian. This is accomplished by enumerating all of the symmetries of the model. The elementary symmetries are \( T, C_{2z}, C_{4z}, T \), and \( C_{2x} \), and \( M_z = TC_{2z} \). We collect their representations and products in Table I. For brevity, we do not include the additional products of other symmetries with \( C_{1z} \) because they are broken if \( C_{1z} \) is broken. Similarly, \( C_{4z} \) is broken if \( C_{2z} \) is broken.

Inversion symmetry \( T \) and \( C_{4z} \) also require composition with other gauge-dependent unitary operators to remain symmetries at \( \phi \neq 0 \). The Landau gauge preserves inversion symmetry. However, the \( 1 \times q \) magnetic unit cell at \( \phi = \frac{2\pi n}{q} \) breaks inversion symmetry. Hence we find that \( T \) acting on the Hofstadter Hamiltonian must be multiplied by a permutation matrix \( D \) that inverts the order of unit cells within the \( 1 \times q \) magnetic unit cell. Explicitly, \( D_{\ell,\ell'} = \delta_{q-\ell,\ell'} \). The Landau gauge explicitly breaks the \( C_{4z} \) symmetry, so a gauge transformation is necessary. In Ref. [50], we will develop the full theory of space group symmetries in the Hofstadter Butterfly. Because we do not use the \( C_{4z} \) symmetry in this work, we refer the reader to Ref. [50] for further details. Considering only the spatial
TABLE I. Symmetries of the BHZ Model

| Symmetry | $\phi = 0$ | $\phi \neq 0$ | Mapping of $k, \phi$ |
|----------|------------|---------------|---------------------|
| $I$      | $I \otimes \tau_3$ | $ID$ | $(-k_x, -k_y, \phi)$ |
| $T$      | $i\sigma_2 \otimes IK$ | $T$ | $(-k_x, -k_y, -\phi)$ |
| $C_{2z}$ | $-i\sigma_3 \otimes \tau_3$ | $(C_{4z}G)^2$ | $(-k_x, -k_y, -\phi)$ |
| $C_{4z}$ | $1/\sqrt{2}(I + C_{2z})$ | $C_{4z}G$ | $(-k_y, k_x, -\phi)$ |
| $M_z$    | $-i\sigma_3 \otimes I$ | $M_z$ | $(k_x, k_y, \phi)$ |
| $C_{2z}$ | $i\sigma_1 \otimes \tau_3$ | $G^{-1}C_{2z}G$ | $(k_x, -k_y, -\phi)$ |
| $M_zC_{2z}$ | $i\sigma_2 \otimes \tau_3$ | $G^{-1}M_zC_{2z}G$ | $(k_x, -k_y, -\phi)$ |
| $TC_{2z}$ | $i\sigma_2 \otimes \tau_3K$ | $TTD$ | $(k_x, k_y, -\phi)$ |
| $TM_zC_{2z}$ | $i\sigma_2 \otimes I$ | $TM_zC_{2z}$ | $(-k_x, k_y, -\phi)$ |
| $TC_{2z}$ | $-i\sigma_3 \otimes \tau_3K$ | $TM_zC_{2z}$ | $(-k_x, k_y, -\phi)$ |
| $TM_zC_{2z}$ | $-I \otimes \tau_3K$ | $TM_zC_{2z}$ | $(-k_x, k_y, -\phi)$ |
| $ITM_zC_{2z}$ | $-i\sigma_3 \otimes IK$ | $ITM_zC_{2z}$ | $(k_x, -k_y, \phi)$ |

We list the symmetries of the BHZ model in column 1 and their representations on the Bloch Hamiltonian in column 2. In column 3, we provide their representations on the Hofstadter Hamiltonian $\mathcal{H}_{QSH}$ in the presence of nonzero flux. The symmetries listed in column 3 refer to the $4 \times 4$ representations defined in column 2. Note that for $\phi \neq 0$, some of the symmetries are broken, and take $\phi \rightarrow -\phi$. The mapping of $k$ and $\phi$ under the action of the symmetries is shown in column 4.

structure and not the orbital character, a generic term in the $\mathcal{H}_{QSH}$ (Eq. (F1)) transforms as

$$
\sum_{\mathbf{R}} C_{4z} \left[ \exp \left( i \int_{\mathbf{R}}^{\mathbf{R} + \mathbf{a}_i} \mathbf{A}(\mathbf{r}) \cdot d\mathbf{r} \right) c_{\mathbf{R} + \mathbf{a}_i}^\dagger \right] C_{4z}^\dagger = \sum_{\mathbf{R}} \exp \left( i \int_{\mathbf{R}}^{\mathbf{R} + \mathbf{a}_i} \mathbf{A}(\mathbf{r}) \cdot d\mathbf{r} \right) c_{\mathbf{R} + \mathbf{a}_i}^\dagger c_{\mathbf{R}} = \sum_{\mathbf{R}} \exp \left( i \int_{\mathbf{R}}^{\mathbf{R} + \mathbf{a}_i} \mathbf{A}(\mathbf{r}) \cdot d\mathbf{r} \right) c_{\mathbf{R} + \mathbf{a}_i} c_{\mathbf{R}} \quad (F5)
$$

This shows us that, because the Peierls phase acquired from the hopping $\mathbf{R} \rightarrow \mathbf{R} + \mathbf{a}_i$ is different from the phase acquired from $C_{4z}\mathbf{R} \rightarrow C_{4z}(\mathbf{R} + \mathbf{a}_i)$, a gauge transformation $G$ is required. We define

$$
Gc_{\mathbf{R},\alpha} G^{-1} = e^{-i\lambda(\mathbf{R})} c_{\mathbf{R},\alpha}, \quad G = \exp \left( i \sum_{\mathbf{R}} c_{\mathbf{R},\alpha}^\dagger c_{\mathbf{R},\alpha} \lambda(\mathbf{R}) \right), \quad (F6)
$$

which acts as a gauge transformation of the vector potential in the Peierls substitution: $Gc_{\mathbf{R} + \mathbf{a}_i,\alpha}^\dagger c_{\mathbf{R},\alpha} G^{-1} = \exp(i \int_{\mathbf{R} + \mathbf{a}_i} \nabla \lambda \cdot d\mathbf{r}) c_{\mathbf{R} + \mathbf{a}_i,\alpha}^\dagger c_{\mathbf{R},\alpha}$. $\lambda(\mathbf{r})$ must satisfy

$$
C_{4z}^{-1} \mathbf{A}(\mathbf{R} + \mathbf{a}_i) - \nabla \lambda(\mathbf{r}) = \mathbf{A}(\mathbf{r}). \quad (F7)
$$

It is trivial to check that $\lambda(\mathbf{r}) = \phi xy$ satisfies Eq. (F7). This completes our discussion of the symmetries.

From Table I, it can be checked that the Hamiltonian with onsite perturbation

$$
H'_{QSH} = H_{QSH} + \epsilon_1 I \otimes \tau_3 + \epsilon_2 \sigma_3 \otimes \tau_2 \quad (F8)
$$

breaks all symmetries except $M_z, T, M_z T$. Thus $H'_{QSH}$ can have no Chern number that would enforce a gap closing, but does still have a Mirror Chern number. If we also add a mirror-breaking term, defining

$$
H''_{QSH} = H'_{QSH} + \epsilon_3 \sigma_2 \otimes \tau_2, \quad (F9)
$$

breaks all symmetries except $M_z, T, M_z T$. Thus $H''_{QSH}$ can have no Chern number that would enforce a gap closing, but does still have a Mirror Chern number.
FIG. 18. We show the Hofstadter Butterfly for $H_{QSH}''$ computed on a $25 \times 25$ unit cell lattice with open boundary conditions along both directions. The model as defined in Table II is in the topological phase and exhibits corner modes (red) that are pumped into the bulk (grey) as $\phi$ is increased.

**TABLE II. QSH Hamiltonians and their Symmetries**

| Hamiltonian | Symmetries | Parameters |
|-------------|------------|------------|
| $H_{QSH}'$ = $H_{QSH} + \epsilon_1 I \otimes \tau_1 + \epsilon_2 \sigma_3 \otimes \tau_2$ | $M_z, T$ | $\epsilon_1 = .1, \epsilon_2 = .11, M = 1.5$ |
| $H_{QSH}'' = H_{QSH} + \epsilon_1 I \otimes \tau_1 + \epsilon_2 \sigma_3 \otimes \tau_2 + \epsilon_3 \sigma_2 \otimes \tau_2$ | $T$ | $\epsilon_1 = .1, \epsilon_2 = .11, \epsilon_3 = .12, M = 1.5$ |
| $H_{QSH}''' = H_{QSH} + \epsilon_4 I \otimes \tau_2 + \epsilon_5 (\sigma_1 + \sigma_2) \otimes I + \epsilon_6 (\sigma_1 \otimes \tau_2 + \sigma_2 \otimes \tau_2 + \sigma_1 \otimes \tau_3)$ | $C_{2z} T$ | $\epsilon_4 = .1, \epsilon_5 = .11, \epsilon_6 = .05, M = 1.6$ |

We list the variations of the BHZ model (column 1), the symmetries they retain from the perturbations (column 2), and the values of the parameters that realize their nontrivial Hofstadter topology (column 3). The Hofstadter Butteryflies of the models may be found in Fig. I and Fig. 18.

then we lose the mirror Chern number and a bulk gap may open (see Fig. I). As demonstrated in Sec., $H_{QSH}''$ – which has only $T$ symmetry – can be classified as a 3D TI with gapless surface states in $\phi$ for open boundary conditions, but it need not have gapless bulk states. Finally, we also can break all symmetries except $C_{2z} T$. Explicitly, we let

$$H_{QSH}''' = H_{QSH} + \epsilon_4 I \otimes \tau_2 + \epsilon_5 (\sigma_1 + \sigma_2) \otimes I + \epsilon_6 (\sigma_1 \otimes \tau_2 + \sigma_2 \otimes \tau_2 + \sigma_1 \otimes \tau_3)$$  \hspace{1cm} (F10)

which preserves $C_{2z} T$ only and opens a gap at all $\phi$. We show the Hofstadter Butlerfly for this model in Fig. 18 and confirm the pumping of corner states that characterizes a HOTI. Note that because $U = 1$ (Eq. (A5)) in our gauge and $H_{QSH}'''$ is identical to $H^{\phi=\pi}$, we trivially have $(UC_{2z} T)^2 = (C_{2z} T)^2 = 1$, which agree with our general calculation in Eq. (E13). We list the values of the parameters in these perturbed Hamiltonians in Table II.

2. Discussion of the Proof for $T$-symmetric TIs with General Flux Periodicity $\phi \rightarrow \phi + 2\pi n$

In this section, we discuss how our proof of the trivial $Z_2$ invariant at $\phi = \Phi/2, \Phi = 2\pi n$ (see Sec.) relies on $n \in \mathbb{N}$ being odd. This leads to a $k_1 \rightarrow k_1 + \pi$ periodicity in the magnetic BZ which ensures every gap closing comes in pairs. If $n$ is even, this proof fails because there is no increased periodicity along $k_1$. In this case, it is unclear a priori whether the $\phi = \Phi/2$ model may be trivial or nontrivial. We show an example of a model with $n = 2$ that can realize either a trivial or nontrivial phase at $\phi = \Phi/2$, confirming that the Hofstadter topology is not uniquely determined by the zero-field topology when $n$ is even.

We begin with the QSH model of App. II. To break the $\Phi = 2\pi$ periodicity to a $\Phi = 4\pi$ periodicity, we add next nearest-neighbor diagonal hoppings as shown in Fig. 19. This term breaks the $\phi \rightarrow \phi + 2\pi$ periodicity because now half a unit cell can be encircled along Peierls paths. However, it does not change $\mu$ because the new hoppings obey $b_1 \cdot ((R + \delta_\phi) - (R' + \delta_\phi)) = b_1 \cdot (a_1 + a_2) = 1$, which does not affect Eq. (A28). We couple $s$ orbitals to $p$ orbitals, preserving $T$ symmetry, and find that in momentum space, the appropriate term is

$$H_{diag}(\mathbf{k}) = \lambda I \otimes \tau_1 (\cos(k_x + k_y) + \cos(k_x - k_y)) .$$  \hspace{1cm} (F11)
We list two variants of BHZ model which realize a weak and strong 3D TI phase (column 1). Each has only $T$ symmetry (column 2). The values of the parameters for these phases are found in column 3.

Consulting App. F we see that this term breaks a number of the zero-field symmetries ($I, C_{2z}, C_{4z}, C_{2x}, M_zC_{2x}, IT, C_{2x}T, C_{2z}T, M_zT, C_{2z}T, M_zC_{2x}T, M_zTC_{2x}, M_zTC_{2z}$) but preserves $T, M_zT, IT, C_{2x}, M_zIT, C_{2x}T, M_zITC_{2x}$. We break all the remaining symmetries except $T$ using the perturbations shown in Table III. The Peierls phase for the two diagonal hoppings are found to be

$$\lambda \to \lambda(\phi) = \lambda \exp\left(i \int_{(x,y)} A \cdot dr \right) = t \exp\left(-i\phi y \pm i\frac{\phi}{2}\right). \quad (F12)$$

At $\phi = 2\pi$ where the new model is $T$ symmetric, the magnetic unit cell is the same as at $\phi = 0$. Indeed, adding the new hopping has not changed $\mu = 1$, thus not requiring an enlarged magnetic unit cell at $\phi = 2\pi$, and the Hamiltonian is the same except for the diagonal coupling which obeys $\lambda(2\pi) = -\lambda$. We now construct two models: $H_{weak}$ is characterized by the parameters $\lambda = -0.1, M = 1.7$ and and $H_{strong}$ is characterized by $\lambda = -0.2, M = 1.85$ (see Table III), each of which has a nontrivial $Z_2$ invariant at $\phi = 0$. We show in Fig. 19 that the first model $H_{weak}$ exhibits a weak Hofstadder TI phase where both the $\phi = 0$ and $\phi = \Phi/2 = 2\pi$ Hamiltonians have nontrivial $Z_2$ invariants, so $\theta = 0$. On the contrary, we show in Fig. 19 that the second model $H_{strong}$ exhibits a strong Hofstadder TI phase where the $Z_2$ invariant at $\phi = \Phi/2$ is trivial, and hence $\theta = \pi$. From these two examples, we see that the topology at $\Phi/2 = n\pi$ cannot be uniquely determined from the $\phi = 0$ topology when $n$ is even, and thus the Hofstadder Hamiltonian may be either a weak or strong TI.

**Appendix G: A Model of Twisted Bilayer Graphene**

In this Appendix, we introduce a model of twisted bilayer graphene on the Moiré lattice. Briefly, we review the fragile topology in zero field, and then we move on to construct the Hofstadder Hamiltonian (App. G1). In App. G2...
we introduce terms that isolate various symmetries of the model, and use these perturbed Hamiltonians to illustrate the results of Sec. We also provide a detailed discussion of the $UC_{2x}T$ symmetry at $\phi = \Phi/2$ and its constraints on the Wilson loop in both the Landau gauge magnetic unit cell and an expanded unit cell (App. G 3). We discuss the bulk gap closings enforced by $C_{2x}$ as mentioned in Sec. and the Wannier flow protected by $C_{2x}T$ from a real space perspective (App. G 4). Finally, we also argue that $C_{2x}T$ can protect a bulk gapless point in App. G 5.

1. The Hofstadter Hamiltonian

In Ref. [8], a 4-band model of twisted bilayer graphene was constructed on the Moiré lattice to capture the phenomenology of the fragile topology inherent to the system. In momentum space, the model is written

$$H_{TBG} (k) = \Delta \mu_3 \otimes \sigma_0 + \mu_0 \otimes \sigma_1 \sum_{i=1}^{3} t \cos(\delta_i \cdot k) + t' \cos(-2\delta_i \cdot k)$$

$$- \mu_0 \otimes \sigma_2 \sum_{i=1}^{3} t \sin(\delta_i \cdot k) + t' \sin(-2\delta_i \cdot k) - 2\lambda \mu_2 \otimes \sigma_3 \sum_{i=1}^{3} \sin(\delta_i \cdot k).$$

Here, $\mu$ (resp. $\sigma$) are the $s, p$ orbital (resp. sublattice) Pauli matrices, and the honeycomb vectors are $a_1 = \sqrt{3}(0, -1)D$, $a_2 = (\frac{1}{2} \sqrt{3})D$ where $D$ is the length of the Moiré superlattice unit cell edge. The nearest-neighbor vectors are $\delta_1 = \frac{1}{3}a_1 + \frac{2}{3}a_2$, $\delta_2 = -\frac{2}{3}a_1 + \frac{1}{3}a_2$, $\delta_3 = \frac{1}{3}a_1 - \frac{2}{3}a_2$, and second-nearest-neighbors are $d_1 = a_1$, $d_2 = a_2$, $d_3 = -a_1 - a_2$. We depict the hopping amplitudes in Fig. [20a]-[20d] and the vectors in Fig. [20e].

Note that for the nearest-neighbor hoppings have two Peierls paths taken in superposition (see Fig. 20f). For example, $C_{2x}$ is the honeycomb cells because, from microscopics, the orbital overlap is greatest there. This is depicted in Fig. 3.

We define the lattice with the center of the honeycomb at the origin, so the orbitals are located at $(r_1 = a_1 + r_2 a_2)$. Following Ref. [8], we choose parameters $t' = -t/3$, $\lambda = \sqrt{2/27}t$ in which case the onsite splitting $\Delta$ determines the topology. For $|\Delta| < 2t$, there is a fragile pair winding of 1 in the Wilson loop of the occupied bands at half filling, which we plot in Fig. 2b. The winding is protected by a $C_{2x}T = I \otimes \sigma_1 K$ symmetry, and the model also has physical $C_{3z} = I, C_{2x} = \mu_3 \otimes I$ symmetries [8]. As written, this model also exhibits the “accidental” symmetries $C_{3z} = I \otimes \sigma_2$ and $C_T = K$ which are separately preserved in the model but need not be preserved in the physical system.

Now we discuss the construction of the Hofstadter Hamiltonian. We proceed in the Landau gauge $A(r) = -\Phi b_1 \cdot b_2$ which we emphasize is centered at the $1a$ position in the center of the honeycomb although there is no orbital there. As argued in Ref. [27], the path of integration of the Peierls phases should be taken through the centers of the honeycomb cells because, from microscopics, the orbital overlap is greatest there. This is depicted in Fig. 3. Calculating the Peierls phases along those paths, we write the model in position space with the magnetic field as

$$H_{TBG}^\Phi = \sum_{\mathbf{R}} \{ e^{i \mathbf{R} \cdot \mathbf{\Delta} \mu_3} \otimes \sigma_0 \mathbf{c}_\mathbf{R} + \sum_{i=1}^{3} \frac{t_i}{2} \mathbf{c}_{\mathbf{R} + \delta_i} \mu_0 \otimes \sigma_1 \mathbf{c}_\mathbf{R} + \frac{t'_i}{2} \mathbf{c}_{\mathbf{R} - 2\delta_i} \mu_0 \otimes \sigma_1 \mathbf{c}_\mathbf{R} + \frac{t'_i}{2} \mathbf{c}_{\mathbf{R} - 2\delta_i} \mu_0 \otimes \sigma_1 \mathbf{c}_\mathbf{R} - \frac{3}{2} \mathbf{c}_{\mathbf{R} + 2\delta_i} \mu_0 \otimes \sigma_1 \mathbf{c}_\mathbf{R} \}$$

where the new hopping elements at each $\mathbf{R} = r_1 a_1 + r_2 a_2$ are calculated using Eq. (A1) and the Peierls paths are given in Fig. 20g,h. We compute the Peierls phases along these paths to be

$$t_i = t \cos \left( \frac{\phi}{6} \right) \left\{ e^{-i \frac{\phi}{2}}, e^{i \frac{\phi}{2}}, e^{i \frac{\phi}{2}}, e^{-i \frac{\phi}{2}} \right\}, \quad t'_i = t' \left\{ e^{i \frac{\phi}{2}}, e^{-i \frac{\phi}{2}}, e^{i \frac{\phi}{2}}, e^{-i \frac{\phi}{2}} \right\},$$

$$\lambda_i = \lambda \left\{ e^{-i \phi (r_2 + 1)}, e^{-i \phi (r_2 + 1)}, e^{i \phi (r_2 + 1)}, e^{i \phi (r_2 + 1)} \right\}.$$

In particular, the nearest-neighbor hoppings have two Peierls paths taken in superposition (see Fig. 20i). For example, the paths $C_1, C_2$ for the $t_1$ hopping are shown in Fig. [21a], and the Peierls substitution reads

$$t_1 \rightarrow t_1(\phi) = \frac{t}{2} \left( e^{i f_{c_1}} A_{-d} + e^{i f_{c_2}} A_{-d} \right)$$

$$= \frac{t}{2} \left( 1 + e^{i f_{c_2} - c_1} A_{-d} \right) e^{i f_{c_1} A_{-d}}.$$
FIG. 20. (a) – (d) We depict the hoppings $t, t'$, and $\lambda$ for the $s$ and $p_z$ orbitals of the model in Ref. [8]. We also show the amplitudes $\epsilon_1, \epsilon_2$, and $\epsilon_3$ of the symmetry breaking terms which are discussed in App. G. For visual clarity, the arrows denoting the hoppings do not correspond to the Peierls paths which are instead shown in Fig. 3. (e) We also depict the first-, second-, and third-nearest neighbor vectors of the model. (f) We show the two Peierls paths of the nearest-neighbor hopping, $C_1$ and $C_2$, we are taken in superposition as we discuss in Fig. 3. (g) We show the second nearest-neighbor path $C_3$. (f) We show the second nearest-neighbor path $C_4$. 

(a)  
(b)  
(c)  
(d)  
(e)  
(f)  
(g)  
(h)
An example of the different atoms in the magnetic unit cell, we derive the Hofstadter Hamiltonian by taking
\[ \phi = \Phi / 2 = 3 \pi, \] the phase difference between \( C_1 \) and \( C_2 \) is equal to \( 3 \pi \times \frac{1}{3} = \pi \) because the paths enclose 1/3 of a unit cell. Thus, their contributions to the amplitude add with exactly opposite signs, and the hopping vanishes. (b) We depict the Peierls paths of the model with the nearest-neighbor hoppings in green, the second nearest-neighbor hoppings in red, and the third nearest-neighbor hoppings in dashed blue. The honeycomb is shown in light grey. We see that any closed loop along the Peierls’ paths encloses an integer number of rhombuses, each of which is 1/3 of the unit cell. Hence \( n = 3 \) and \( \Phi = 6 \pi \). (c) We show the 1 \times 2 magnetic unit cell of the model at \( \phi = \mu \frac{2 \pi p}{q} = \frac{3 \pi}{2} \) outlined in dotted grey lines. In addition for visual clarity, we also show examples of the first-, second-, and third nearest neighbor paths shown with the same colors as in (b).

Noting that \( C_2 - C_1 = \partial \mathcal{R} \), where \( \mathcal{R} \) is marked as the grey rhombus in Fig. 21, is a closed loop of area 1/3 (recalling that have normalized the area of the unit cell to 1), we find
\[
t_1(\phi) = \frac{t}{2} \left( 1 + e^{i\phi/3} \right) \left( e^{i \int_{C_1} A \cdot dr} e^{i \frac{2}{3} \int_{C_1} A \cdot dr} \right) = \frac{t}{2} \left( e^{-i \phi/6} + e^{i \phi/6} \right) \left( e^{i \frac{2}{3} \phi} + e^{i \frac{2}{3} \phi} \right) = t \cos \left( \frac{\phi}{3} \right) e^{i \frac{2}{3} \phi} \int_{C_1} A \cdot dr.
\]

Computing the remaining integral gives Eq. (G3). We emphasize in the \( \lambda \) hopping term, \( \sigma_z \to \text{diag}(\lambda, -\lambda') \) because the different sublattice sites have different hopping paths. We refer to the phases of the hoppings as \( \arg t_i = \varphi_{r1}(\ell) \), \( \arg t_{i'} = \varphi_{r1}(\ell) \), \( \arg \lambda_i = \varphi_{\lambda i}(\ell) \), \( \arg \lambda_{i'} = \varphi_{\lambda i}(\ell) \).

To Fourier transform Eq. (G2) in momentum space in the Landau gauge, we compute \( \mu \) using Eq. (A28). To do so, we only need the vectors between orbitals connected by hoppings, which for nearest neighbors are \( \delta_1 \), second nearest neighbors are \( \delta_2 \), and third nearest neighbors are \( -2\delta_3 \). From Eq. (A28), we calculate \( \mu = \text{lcm} \{ b_1 \cdot \delta_1, b_1 \cdot \delta_2, b_1 \cdot (\delta_1 + (2\delta_3)) \} \) = \{ 1, 3, -1/3, 1/3, 1, 0, -\frac{2}{3}, \frac{2}{3}, -\frac{2}{3} \} = 3. Hence, we can form the Hofstadter Hamiltonian by taking \( \phi = 3 \frac{2 \pi p}{q} \) for \( p', q' \) coprime, and define the magnetic BZ as \( k_1 \in (-\pi, \pi), k_2 \in (0, \frac{2 \pi}{q'}) \) with a 1 \times \frac{q'}{2} magnetic unit cell. Indeed, one can check that \( \phi = 3 \frac{2 \pi p}{q} \) explicitly gives a \( r_2 \to r_2 + q' \) periodicity in the Peierls phases from Eq. (G3).

Note that in Ref. [37], the Hofstadter of the model was constructed in the square lattice gauge \( A_{bq}(r) = \phi(0, x) \), which is not the form of our Landau gauge, \( A(r) = -\phi b_1(r \cdot b_2) \). In the square lattice gauge, Ref. [37] found it was necessary to rationalize the flux as \( \phi = 2 \frac{2 \pi p}{q} \). There is no contradiction because the rationalization is gauge-dependent.

The flux periodicity \( \Phi \) is gauge invariant and is determined by the possible loops along Peierls paths. We overlay all possible Peierls paths in Fig. 21, from which we can see that all paths enclose a multiple of 1/3 of a unit cell. Hence \( n = 3 \) and \( \Phi = 6 \pi \). Note that \( \mu \) and \( n \) being identical is coincidental, as can be seen by considering the gauge choice of Ref. [37] where this explicitly does not hold.

We now construct the Hofstadter Hamiltonian. As required, there is no dependence on \( r_1 \) and the Hamiltonian can be Fourier transformed over \( a_1 \) immediately. At \( \phi = 3 \frac{2 \pi p}{q} \), we choose the unit cell to be indexed by \( \ell = 0, \ldots, q' - 1 \). An example of the \( \phi = 3 \pi \left( q' = 2 \right) \) magnetic unit cell is shown in Fig. 21. Keeping track of how the hoppings connect different atoms in the magnetic unit cell, we derive the Hofstadter Hamiltonian
\[
[H^\phi(k)]_{\ell, \ell'} = \delta_{\ell \ell'} \h_\ell + \delta_{\ell-1, \ell} T_\ell + \delta_{\ell', -1, \ell} T_{\ell'} + \delta_{\ell', -2, \ell} S_{\ell} + \delta_{\ell', -2, \ell} S_{\ell'}
\]
TABLE IV. Symmetries of the TBG Model

| Symmetry | $\phi = 0$ | $\phi \neq 0$ | Mapping of $k, \phi$ |
|----------|------------|------------|-------------------|
| $C_{3z}$ | $I$        | $C_{3z}G_{2z/3}$ | $R_{2z/3}k, \phi$ |
| $C_{2z}$ | $\mu_3 \otimes I$ | $C_{2z}$ | $(k_x, -k_y), -\phi$ |
| $T$      | $K$        | $T$        | $-k_x, -\phi$ |
| $C_{2z}T$ | $I \otimes \sigma_1$ | $C_{2z}D$ | $-k_x, \phi$ |

We list the symmetries of the TBG model Eq. (G2) in column 1 and their representations on the Bloch Hamiltonian $H_{TBG}$ in column 2. In column 3, we provide their representations on the Hofstadter Hamiltonian $H_{TBG}'$ in the presence of nonzero flux. The symmetries listed in column 3 refer to the $4 \times 4$ representations defined in column 2. Note that for $\phi \neq 0$, some of the symmetries are broken, and take $\phi \rightarrow -\phi$. The mapping of $k$ and $\phi$ under the action of the symmetries is shown in column 4.

where the $4 \times 4$ blocks are given by

$$h_{\ell} = \frac{\Delta \mu_3}{2} \otimes \sigma_0 + \mu_3 \otimes \sigma_1 \left[ |t_{\ell}| \cos(k \cdot \delta_1 - \varphi_{1\ell}(\ell)) + t' \cos(2k \cdot \delta_2 + \varphi_{t2}(\ell)) + t' \cos(2k \cdot \delta_3 + \varphi_{t3}(\ell)) \right]$$

$$- \mu_3 \otimes \sigma_2 \left[ |t_{\ell}| \sin(k \cdot \delta_1 - \varphi_{1\ell}(\ell)) + t' \sin(-2k \cdot \delta_2 - \varphi_{t2}(\ell)) + t' \sin(-2k \cdot \delta_3 - \varphi_{t3}(\ell)) \right]$$

$$- \lambda \mu_2 \otimes \text{diag}(\sin(k \cdot d_1 - \varphi_{1\ell}(\ell)), -\sin(k \cdot d_1 - \varphi_{1\ell}(\ell)))$$

$$T_{\ell} = \mu_0 \otimes \sigma_1 - i \mu_0 \otimes \sigma_2 \left[ e^{i\varphi_{1\ell}(\ell)} e^{-i\hbar k} + e^{i\varphi_{t2}(\ell)} e^{-i\hbar k} \right]$$

$$- i \lambda \mu_2 \otimes \left( -\text{diag}(e^{-i\hbar k}, -e^{i\hbar k}) e^{ikd_2} + \text{diag}(e^{i\hbar k}, -e^{i\hbar k}) e^{-ikd_2} \right)$$

S_{\ell} = \frac{t'}{2} \left( \mu_0 \otimes \sigma_1 - i \mu_0 \otimes \sigma_2 \right) e^{i\varphi_{t2}(\ell) + 2ikd_1}.

This completes the construction of the Hofstadter Hamiltonian. We can now discuss the symmetries of the $H_{TBG}'$ at nonzero flux. The $\phi = 0$ symmetries are promoted to those in Table IV (third column) when $\phi \neq 0$ with the additional $D$ and $G'$ factors. For brevity, we do not include product symmetries with $C_{3z}$ and the other symmetries since they are broken when we break $C_{3z}$. Again, $D_{\ell'} = \delta_{\ell, \ell'} - \ell'$ acts on the (enlarged) magnetic unit cell indices to flip the magnetic unit cell under $C_{2z}$. Additionally, $C_{3z}$ requires a gauge transformation because our Landau gauge explicitly breaks $C_{3z}$ symmetry. To determine the appropriate gauge transformation $G'$, we refer to the discussion around Eq. (F5) which shows that

$$G' = \exp \left( \sum_{\mathbf{R}_0} i \mathbf{c}_{\mathbf{R}_0} \mathbf{c}_{\mathbf{R}_0} \mathbf{\chi}(\mathbf{R} + \delta_\alpha) \right)$$

where $\mathbf{\chi}(\mathbf{r}) = -\phi xy$ is the solution to

$$C_{3z}^{-1} \mathbf{A}(C_{3z} \mathbf{r}) - \nabla \mathbf{\chi}(\mathbf{R}) = \mathbf{A}(\mathbf{r}).$$

We refer the reader to Ref. [50] for a detailed treatment of space group symmetries in the presence of magnetic fields. We note that there is also a particle-hole symmetry $Ph = \mu_1 \otimes \sigma_3$ that obeys

$$Ph H_{TBG}(k) Ph = -H_{TBG}(k)$$

which exists at $\phi = 0$ and $\phi = \Phi/2$.

Using these expressions, one can check explicitly that the symmetries in Table IV are preserved. For symmetries that take $\phi \rightarrow -\phi$, the zero-field symmetry is restored at $\Phi/2 = 3\pi, \phi' = 1/2$. At this point, cos $\Phi/2 = 0$, so nearest neighbor couplings vanish due to the interference of their Peierls paths. Fig. 21 illustrates that the phase difference between the two paths is $\pi$, and they destructively interfere.

2. Breaking Symmetries

Like in the case of the QSH model, we may add symmetry-breaking terms to $H_{TBG}$ in order to isolate the effects of various symmetries. In Sec. , we showed that $C_{2z}T$ symmetry alone was responsible for the HOTI classification...
of the Hofstadter phase, and thus we build perturbations to destroy all other symmetries of the model. By coupling nearest neighbor atoms with an imaginary coupling that takes opposite signs for the $s$ and $p_z$ orbitals, we break $C_{2z}$ and $T$ symmetry individually. In momentum space at $\phi = 0$, this term reads

$$H_1(k) = \mu_3 \otimes \sum_i (\sigma_1 \sin \delta_i \cdot k + \sigma_2 \cos \delta_i \cdot k). \quad (G11)$$

One may check that this term breaks $C_{2z}, T, C_{2z}T, C_{2z}C_{2z}$. To break $C_{3z} = I \otimes I$, we add an anisotropic term that alters only the $\delta_1$ hopping,

$$H_2(k) = \mu_0 \otimes (\sigma_1 \cos \delta_1 \cdot k - \sigma_2 \sin \delta_1 \cdot k). \quad (G12)$$

To break $C_{2z}$ and all the remaining product symmetries, we use the term

$$H_3(k) = \mu_1 \otimes \sum_i (\sigma_1 \cos \delta_i \cdot k - \sigma_2 \sin \delta_i \cdot k). \quad (G13)$$

One may check that all these perturbations preserve the particle-hole symmetry Eq. (G10). This is desirable for stabilizing the corner modes at zero energy, although this is not essential to the physics of the model. We will show in App. [G4] that if $C_{2z}$ and $T$ are maintained, then a bulk gap closing is enforced by the $C_{2z}$ eigenvalues. To show this, we remove $H_1$ to create the Hamiltonian $\tilde{H}_T'_{TBG}$ which possesses $C_{2z}, T$, and their product $C_{2z}T$. $\tilde{H}_T'_{TBG}$ has a gapless bulk due to $C_{2z}$ (see Fig. 23). Note that although $\tilde{H}_T'_{TBG}$ has a $T$ symmetry, this model is spinless and thus $T^2 = +1$ so there is no Kane-Mele invariant. The models in this section are summarized in Table V.

### 3. Computing the $w_2$ index protected by $UC_{2z}T$ symmetry

From Table V, we see that $\tilde{H}_T'_{TBG}$ has a $C_{2z}T$ symmetry and hence has $UC_{2z}T$ symmetry at $\phi = \Phi/2$. As shown in Fig. 15a, ($UC_{2z}T)^2 = e^{i\pi/2}(C_{2z}T)^2 = +1$, so the phase at $\phi = \Phi/2$ is characterized by the $w_2$ invariant. Following the discussion of App. [G2], where we used this model as an example, we can compute this invariant in a $2 \times 2$ unit cell where $UC_{2z}T$ acts diagonally in momentum space. For pedagogical purposes, we also compute the Wilson loop in the $1 \times 2$ unit cell at $\phi = \Phi/2$ where $UC_{2z}T$ is not diagonal and there is no particle-hole symmetry in the Wilson spectrum. We plot the Wilson loop spectra using these two possible unit cells in Fig. 22. From the spectrum of Fig. 22b, we observe that there are no crossings at $\theta = 0$ or $\theta = \pi$ and thus $w_2^{\phi=\Phi/2} = 0$. Note that the number of crossings at $\theta = 0$ must equal the number at $\theta = \pi$ because $\{\theta(k_1 + \phi)\} = \{\theta(k_1) + \pi\}$ (see Eq. (C12)). From here, we can calculate the Hofstadter HOTI invariant

$$\theta = w_2^{\phi=0} - w_2^{\phi=\Phi/2} = 1 \quad (G14)$$

recalling that $H^{\phi=0}$ is nontrivial. Thus corner states are pumped into the bulk as the flux is tuned from 0 to $\Phi/2$ as we see in Fig. 21 of the Main Text. We discuss the signatures of this phase in the following section App. [G4] from a real-space perspective.

### 4. $C_{2z}$ Symmetry Eigenvalues

When $C_{2z}$ and $T$ remain symmetries of the model as in $\tilde{H}_T'_{TBG}$, a gap closing may be enforced by the symmetry eigenvalues of $C_{2z}$, as we observe from the Hofstadter Butterfly in Fig. 23. We will prove this gap closing for $\tilde{H}_T'_{TBG}$.

| Hamiltonian | Symmetries | Parameters |
|-------------|------------|------------|
| $H_{TBG}'$ = $H_{TBG} + \epsilon_1 H_{1,1w}(k) + \epsilon_2 H_{2}(k) + \epsilon_3 H_{4}(k)$ | $C_{2z}T$ | $\epsilon_1 = .12, \epsilon_2 = .11, \epsilon_3 = .1, \Delta = 1.6$ |
| $H_{TBG}'' = H_{TBG} + \epsilon_2 H_{2}(k) + \epsilon_3 H_{4}(k)$ | $C_{2z}, T, C_{2z}T$ | $\epsilon_2 = .11, \epsilon_3 = .1, \Delta = 1.6$ |
| $H_{TBG}''' = H_{TBG} + \epsilon_2 H_{2}(k) + \epsilon_4 H_{4}(k)$ | $C_{2z}T$ | $\epsilon_2 = .11, \epsilon_4 = .1, \Delta = 1.6$ |
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FIG. 22. (a) We show the Wilson Loop spectrum for $H'_{TBG}$ in the $1 \times 2$ magnetic unit cell of our Landau gauge at $\phi = \Phi/2$ where $UC_{2z}T$ is not diagonal in momentum space. Hence there is no “particle-hole” symmetry. (b) To make $U$ diagonal in momentum space such that the Wilson spectrum realizes the “particle-hole” symmetry of a conventional $w_2$ insulator, we diagonalize $H^{\Phi/2}_{TBG}$ in a $2 \times 2$ unit cell where $k_1$ is defined in $(-\pi/2, \pi/2)$. We calculate the Wilson loop for this Hamiltonian and observe that it matches the spectrum of (a) with the Wilson bands folded so $k_1$ is defined only mod $\pi$. Note that $(UC_{2z}T)^2 = +1$, so we may calculate $w^{\phi=\Phi/2}_{2}$ as described in App. E2 without calculating the nested Wilson loop.

FIG. 23. The Hofstadter Butterfly is calculated on a $20 \times 20$ lattice in the topological phase for $H''_{TBG}$, described in App. G1, which has both $C_{2z}$ and $T$. Because $C_{2z}T$ remains, there is still corner mode pumping, but the model is not a HOTI due to the bulk gap closing enforced by $C_{2z}$ eigenvalues. We demonstrate this in (b) and (c), where the Wannier centers of the phases at $\phi = 0, 3\pi$ are shown in red and blue respectively in magnetic unit cell. (We show the boundary of the standard unit cell and its $1c, 1d$ orbitals with dashed lines.) A possible Wannierization is shown in (b), with $s$ and $p_z$ orbitals at the $1b$ and $1c$ positions. Without breaking $C_{2z}$ symmetry, pairs of orbitals may be moved to other high symmetry Wyckoff positions, but it is impossible to reach the state at $\phi = 0$.
(see Table VII using the framework of Topological Quantum Chemistry [60][62]. To obtain the band representations of this model, we calculate the $C_2$ eigenvalues directly from $H''_{TBG}$ (see Table VII) for $\phi = 3\pi$ at the 4 inversion invariant points in the $\phi = 3\pi$ BZ. The calculation is straightforward at $\phi = 3\pi$ using the embedding matrices and symmetries defined in Sec. A8 and App. G1, respectively. At $\phi = 0$, note that we must artificially extend the $1 \times 1$ unit cell to the $1 \times 2$ magnetic unit cell to compare the atomic limits of the band representations at $\phi = 0$ and $\phi = 3\pi$ in the same unit cell.

We collect the eigenvalues of the occupied bands in Table VII. We note that at $\phi = 0$ and $\phi = 3\pi$, all bands are connected energetically. We emphasize that Wyckoff positions correspond to the magnetic unit cell, i.e. $1a = (0,0), 1b = a_1/2, 1c = 2a_2/2, 1d = a_1/2 + 2a_2/2$ taking the center of the hexagonal plaquette (1a) as the origin.

![Table VI. TBG $C_2$ eigenvalues](image)

| $\xi^{\phi=0}$ | $\pi b_1$ | $\pi b_2$ | $\pi b_1 + \pi b_2$ | Band Representation |
|----------------|---------|---------|--------------------|--------------------|
| $-1,-1,1,1$   | $B^{\phi=0} = 2\Gamma_1 + 2\Gamma_2 + 4\Gamma_1 + 2\Gamma_1 + 2\Gamma_2 + 2\Gamma_4 + 2\Gamma_4 + 2\Gamma_4$ |
| $\xi^{\phi=3\pi}$ | $-1,-1,1,1$ | $B^{\phi=3\pi} = 2\Gamma_1 + 2\Gamma_2 + 2\Gamma_1 + 2\Gamma_2 + 2\Gamma_1 + 2\Gamma_2 + 2\Gamma_4 + 2\Gamma_4 + 2\Gamma_4$ |

In columns 1-4, we show the $C_2$ eigenvalues calculated from $H''_{TBG}$ (see Table VII) at half filling in the $1 \times 2$ magnetic unit cell at both $\phi = 0$ and $\phi = 3\pi$. Column 5 shows the (spinless) band representations determined from the eigenvalues.

We see that we may obtain the momentum space band representations of Table VII by inducing orbital atoms from high symmetry Wyckoff positions to the full space group [63][64]. First we consider the $\phi = 0$ band representation. Because no $B_2$ irreps appear, the possible atomic orbitals are $A_{1a}, B_{1b}, A_{1c}, B_{1d}$, recalling that $A(B)$ is the even (odd) irrep under $C_2$. There is only one Wannierization possible:

$$BR^{\phi=0} = (A_{1a} \oplus B_{1b} \oplus A_{1c} \oplus B_{1d}) \uparrow G.$$  \hspace{1cm} (G15)

We show the location of the Wannier centers in Fig. 23a.

Next, we consider the bands at $\phi = 3\pi$ forming $BR^{\phi=3\pi}$. In this case, there are many non-unique atomic limits that recover the band structure. Note that any pair of locally even irreps (s orbitals) and locally odd irreps (p$_z$ orbitals) at the same Wyckoff position $w$ yields the band representation $(A_w \oplus B_w) \uparrow G = \Gamma_1 + \Gamma_2 + B_1 + B_2 + Y_1 + Y_2 + A_1 + A_2$ when induced to the space group. Thus placing both an s and p$_z$ orbital at any two high symmetry Wyckoff positions $w_1, w_2$ will yield $(A_{w_1} \oplus B_{w_1} \oplus A_{w_2} \oplus B_{w_2}) \uparrow G = BR^{\phi=3\pi}$. In fact, these limits $A_{w_1} \oplus B_{w_1} \oplus A_{w_2} \oplus B_{w_2}$ are the only possible atomic limits. This may be shown by exhaustion. In Fig. 23b, we show one such Wannierization to the $1b$ and $1c$ Wyckoff positions within the magnetic unit cell.

We conclude that there must be an odd number of irreps at the $1a$ position for $\phi = 0$, but there must be an even number of irreps at the $1a$ position for $\phi = 3\pi$. Under $C_2$-preserving perturbations that preserve the gap, electrons may be moved off the high symmetry Wyckoff positions into the $2c = (x,y),(1-x,1-y)$ position in pairs, so necessarily only an even number of electrons can be deformed to another high symmetry Wyckoff position. We see that $BR^{\phi=0}$ and $BR^{\phi=3\pi}$ are incompatible in this manner, and a gap closing must occur at an intermediate $\phi$ while $C_2$ is preserved, as we see in Fig. 23a. We underscore that although the magnetic unit and the magnetic BZ do not evolve smoothly as the flux is increased, the Wannier centers do evolve smoothly, which our argument relies on.

We can also use this position-space argument to understand the Wannier flow that characterizes the Hofstadter HOTI phase when $C_{2z}$ is broken but $C_{2z}T$ is preserved. For instance, we can take $H''_{TBG}$ and break its $C_{2z}$ symmetry by adding a small perturbation Eq. (G11), resulting in the new model $H''_{TBG}$ which only has $C_{2z}T$ symmetry. Let us first consider the Wannier centers of $H''_{TBG}$ at $\phi = 0$ and $\phi = 3\pi$ where $UC_{2z}T$ still pins Wannier centers to the high-symmetry Wyckoff positions (which are invariant under the magnetic point group $2'$ (a proper subset of the point group 2) symmetries). Then as argued in App. G3 the Wannier centers must flow nontrivially between $\phi = 0$ and $\phi = 3\pi$ where there are different Wannierizations. However, with $C_{2z}$ broken, this Wannier flow does not require a gap closing as the flux is tuned from 0 to 3$\pi$. This is because the Wannier centers are not constrained to obey $C_{2z}$ symmetry at all $\phi$. Instead, the Wannier flow is $C_{2z}T$-symmetric: if there is a Wannier center at $r$ at flux $\phi$, then by $C_{2z}T$, there is a Wannier center at $-r$ and $\phi$. So each trajectory $r(\phi)$ must obey $r(\phi) = -r(-\phi)$. Thus as we tune the flux through its full period, we find nontrivial Wannier flow that pumps electrons between unit cells. We depict an example in Fig. 24 of two electrons interpolating between the $1a, 1d$ Wyckoff positions at $\phi = 0$ and the $1c, 1b$ positions at $\phi = \Phi/2$. On open boundary conditions, this induces corner state flow. The corner states must be degenerate in energy at $\phi = 0$ because they are $C_{2z}T$ partners, and are pinned to zero energy when particle-hole symmetry exists. As the flux is increased, the pumping converts an occupied energy level to a hole on one of the boundaries with the reverse process happening on the other boundary by $C_{2z}T$, matching the energy splitting in Fig. 2.
FIG. 24. (a) We show an example of $C_{2x}T$ symmetric Wannier flow from $\phi = -3\pi$ to $\phi = 3\pi$, going from the 1b, 1c positions at $\phi = -3\pi$ (blue) to the 1a, 1d positions (red), and back to the 1b, 1c positions at $\phi = 3\pi$. When we break $C_{2x}$, the orbitals may move slightly from the maximal Wyckoff positions. However, with $C_{2x}T$ intact, the Wannier flow is still protected. (b) We show the Hofstadter Butterfly for $H''_{TBG}$ on periodic boundary with only $C_{2x}T$ symmetry, and observe the bulk gap closing. The exact Hamiltonian is given in Table V. Because $C_{2x}T$ is broken, there is also no $w_2^{\phi=a}$ invariant to protect winding in the Wilson loop. Thus the Hofstadter Topology is trivial, although the the bulk gap closing at finite flux is locally protected by $C_{2x}T$.

5. $C_{2x}T$-Protected Gap Closing

While we have not paid much attention to the $C_{2x}$ and $C_{3z}$ symmetries of the model, it is important to break the composite symmetry $C_{2x}T$ to realize the HOTI phase. (Note $C_{2x}T$ exists in $H_{TBG}$ due to the accidental $T$ symmetry.) We argue now that because both $C_{2x}$ and $T$ take $\phi \to -\phi$ in the Hofstadter Hamiltonian (see Table IV), $C_{2x}T$ is preserved at all flux and may protect a gap closing [65].

Let $H^\phi(k)$ be the Hofstadter Hamiltonian of the $H_{TBG}$. It obeys

$$C_{2x}T H^\phi(k_x, k_y)(C_{2x}T)^{-1} = H^\phi(-k_x, k_y), \quad C_{2x}T = I_{q'} \otimes (-i\mu_3 \otimes I_3 K),$$

with $I_{q'}$ the $q' \times q'$ identity matrix. Our strategy for understanding the bulk gap closing is to study an effective two band Hamiltonian that models the low energy behavior near the Fermi level. We will show that generically, $C_{2x}T$ symmetry is sufficient to prove a gap closing between the two bands at some $\phi$, but this is only a proof of local stability. In particular, the assumption of an effective two band model assumes the two bands are close to each other and well separated from all other bands. This is certainly false when $\Delta$, the onsite potential, is large and the conduction bands are far from the valence bands. As such no gap closing need exist. This is similar to the local stability of a Weyl node, which is locally protected but can be gapped out in pairs.

Because $C_{2x}T$ acts as the identity on the sublattice index but as $-i\mu_3$ on the spin indices (see Eq. (G16)), the minimal low energy Hamiltonian consists of two bands which adequately models the highest energy valence band and lowest energy conduction band. The most general effective Hamiltonian is then

$$H_{eff}(k_x, k_y, \phi) = d_0(k, \phi)\mu_0 + d_1(k, \phi)\mu_1 + d_2(k, \phi)\mu_2 + d_3(k, \phi)\mu_3$$

and acting on this Hamiltonian, $C_{2x} = -i\mu_3 K$. At $k_x = 0$, Eq. (G16) mandates that $C_{2x}T$ commute with $H_{eff}$ at all $k_y, \phi$. Using Eq. (G17), we compute

$$C_{2x}T H_{eff}(0, k_y, \phi)(C_{2x}T)^{-1} = d_0(0, k_y, \phi)\mu_0 - d_1(0, k_y, \phi)\mu_1 + d_2(0, k_y, \phi)\mu_2 + d_3(0, k_y, \phi)\mu_3 .$$

But $[C_{2x}T, H_{eff}(0, k_y, \phi)] = 0$, so $d_1 = 0$. There are two free parameters, $k_y \in (-\pi, \pi), \phi \in (0, 6\pi)$, which we fix by the requirement that $d_2(0, k_y^*, \phi^*) = d_3(0, k_y^*, \phi^*) = 0$. Generically, such a $k_y^*$ and $\phi^*$ will exist because the $d_1, d_2$ space is of codimension 0. In this case, $H_{eff}(0, k_y^*, \phi^*) \propto \mu_0$, and the two bands must be degenerate in energy.
We substantiate this argument with a numerical calculation of the Hofstadter Butterfly. We build $H''_{TBG}$ by adding terms to $H_{TBG}$ that break all symmetries except $C_{2x}T$. We make use of the new perturbation

$$H_4(k) = \mu_0 \otimes \sigma_3 + \mu_2 \otimes \sigma_0 + \mu_3 \otimes \sigma_3$$

which is onsite and preserves $C_{2x}T$. Explicitly, it breaks $C_{2z}, C_{2x}, T, C_{2z}T, C_{2z}C_{2z}, C_{2z}C_{2z}T$, and particle-hole symmetry. Using these perturbations, we build $H''_{TBG} = H_{TBG} + \epsilon_2 H_2(k) + \epsilon_4 H_4(k)$ and include precise values of the parameters in Table V. We show the spectrum in Fig. 24b and observe that the bulk is gapless due to the Weyl node at $(k_x, k_y, \phi) = (0, k_y^*, \phi^*)$. 
