π -fluxes, semimetals, and flat bands in artificial materialsToshikaze Kariyado^{1,2} and Robert-Jan Slager²¹*International Center for Materials Nanoarchitectonics (WPI-MANA), National Institute for Materials Science, Tsukuba, Ibaraki 305-0044, Japan*²*Department of Physics, Harvard University, Cambridge, Massachusetts 02138, USA*

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The possibility of engineering experimentally viable systems that realize gauge fluxes within plaquettes of hopping has been the subject of a search for decades due to vast amounts of theoretical study. This is of particular interest for topological band insulators, where it is known that such fluxes bind protected midgap states. These modes can hybridize in extended flux lattices, giving rise to semimetallic bands that are highly tunable. We demonstrate that within artificial materials, local π -fluxes can be naturally realized. Also, the importance of the crystalline symmetry for protecting the π -flux modes is pointed out. Consequently, we provide concrete setups and conditions to access this physics and analyze similar self-organized band structures and physical properties. Our work therefore not only pinpoints simple systems exhibiting flat bands but also opens up a route to study flux lattice models and associated effective theories.

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Introduction. Gauge fluxes have been associated with many exotic physical properties studied over several decades, from, e.g., vortices in lattice gauge theories [1] to quasiparticle descriptions in quantum Hall systems [2]. Similarly, topological band insulators [3,4], arising by virtue of interplay between symmetry and topology [5–15], or symmetry-protected states in general [16–18], can be unambiguously distinguished from trivial states by monodromy defects [19–24], i.e., effective gauge fluxes. Such defects bind modes that relate to the relevant topological invariants [25–28].

Despite the richness of such theoretical insights, realizing gauge fluxes in accessible setups is still a standing question. The difficulty here mainly is the condition that the mentioned model settings require fluxes that are localized to one or a few plaquette(s) of hopping sites. Although intriguing proposals utilizing the controllability of cold atom systems [29,30] or vortex lattices in type-II superconductors [31] may become within reach over time, such experiments will unavoidably be involved. This in some sense also applies to routes that use lattice defects to act as effective fluxes [21,32–35]. While recent experimental results in fact seem promising [36], controlling and manipulating defects will require additional progress.

In this work, we analyze physical consequences of localized fluxes within the context of readily controllable artificial materials. We retrieve π -flux bound midgap zero modes in topological regimes, as in electronic counterparts. Apart from providing concrete setups, we show that in extended flux

lattices these modes hybridize into midgap band structures that have gapless touching points at specific points in the Brillouin zone. This leads to transport features of the highly tunable bands that can readily be flattened by increasing the spacing of the flux lattice. Given the implementability of the outlined structures, this opens the door to studying gauge flux models in a controllable setups and harvesting the associated rich physics and potential applications, for instance, realized by coupling interface-edge states with π -flux states.

Model. To make our arguments concrete, we analyze band dispersions of a modulated honeycomb lattice tight-binding model with π -flux lattice on top of it. We consider the simple Hamiltonian $H = \sum_{\langle ij \rangle} t_{ij} c_i^\dagger c_j$, where $\langle ij \rangle$ refers to the nearest neighbors and $c_i^\dagger$ is the creation operator at site i . Furthermore, the hopping parameters t_{ij} are set in terms of modulations of the type depicted in Fig. 1, in which we assign intrahexagon hopping $t_0 = t + \delta$ for black bonds and interhexagon hopping $t_1 = t - \delta$ for red bonds. This modulation gaps out Dirac cones of the original honeycomb lattice model through the coupling between the Dirac cones at the K and K' points in the Brillouin zone [27]. Importantly, the states near zero energy are known to be described by a massive Dirac equation where the sign of the mass term can be flipped by changing the ratio between $|t_0|$ and $|t_1|$ or the sign of δ . The feature that the sign flip of the mass term can be induced by a little modulation in the hopping amplitude makes this model an ideal playground to simulate a quantum spin Hall state in artificial systems. Indeed, several of the experimental demonstrations of helical edge states in the literature in fact implement this model [37–45]. This δ -induced gapped phase has also been analyzed from a topological crystalline insulator viewpoint [46–48]. In the following, we set $t = -1$, and $|\delta| = 0.1$. Note that $\delta > 0$ corresponds to $|t_0| < |t_1|$ while $\delta < 0$ corresponds to $|t_0| > |t_1|$. Throughout the paper, we use a_0 as the nearest neighbor distance between the sites in the honeycomb lattice.

FIG. 1. (a) Schematic picture for the modulated honeycomb lattice model with π -flux. The hopping amplitude is different on the black and the red bonds. The shaded hexagons are threaded by π -flux. [(b), (c)] Corresponding π -flux strings. The strings in panels (b) and (c) are gauge related.

To implement a π -flux lattice, we pick up two hexagons and connect them by a string that flips the sign of the hopping on the intersecting bonds. There is arbitrariness in the path of the strings, i.e., if two strings form a loop when they are combined, the two ways are related by a gauge transformation and physically equivalent. For instance, Figs. 1(b) and 1(c) are physically the same. Note that a periodic supercell has to contain even number of π -flux threaded hexagons. In the following, when we see the band structure as a function of k_x , we implicitly chose the string alignment as in Fig. 1(c) to minimize the period in the x direction, while when we see the band structure as a function of k_y , the alignment in Fig. 1(b) is chosen to minimize the period in the y direction.

Because of the hopping modulation, hexagons in the current model can be classified into two kinds; one consists of the black bonds exclusively, while the other consists of the mixture of the black and red bonds. We first consider the case where the π -fluxes are placed on the hexagon of the first kind, as in Fig. 1, and check the existence of the midgap states by looking at the isolated π -flux. In practice, we numerically obtain the energy spectrum and the wave functions with sufficiently large L_x and L_y . A clear sign of the midgap state is found for $|t_0| > |t_1|$. There appear two bound states per a π -flux, whose wave functions are shown in Fig. 2.

For the case with $L_x \ll L_y$, the system is essentially regarded as a one-dimensional π -flux lattice (π -flux chain) along the zigzag direction, while for the case with $L_x \gg L_y$, the system is regarded as a π -flux chain along the armchair direction. In such cases, we can think of band structures generated by hybridizations between the bound states of the

FIG. 2. Wave functions for the two midgap states bound to an isolated π -flux marked as a cyan hexagon. The size of each of the disks represents the amplitude of the wave function at the corresponding site, while the color (orange or blue) is for the sign of the wave function. $L_x = 36\sqrt{3}a_0$ and $L_y = 72a_0$ are adapted and the gauge in Fig. 1(c) is used.

FIG. 3. (a) Band structure for $L_x = 3\sqrt{3}a_0$ and $L_y = 36a_0$. With this setup, the π -flux threaded hexagons essentially align in the zigzag direction, and the focus is on the band dispersion along that direction. (b) Band structure for $L_x = 12\sqrt{3}a_0$ and $L_y = 6a_0$. The focus is on the band dispersion along the armchair direction. [(c), (d)] Energy gap across the zero energy at $k_{x,y} = 0$. (c) L_y dependence for several choices of L_x , proving the gapless nature. (d) L_x dependence for several choices of L_y , detecting finite minigap not from the size effect.

neighboring π -fluxes. The results for $L_x \ll L_y$, i.e., the band structures of the π -flux chain along the zigzag direction, are shown in Fig. 3. We clearly see an in-gap state with one-dimensional (1D) Dirac structure at the zone center and the corner for $|t_0| > |t_1|$, while no in-gap state for $|t_0| < |t_1|$ is retrieved. Similar band structures are obtained also for $L_x \gg L_y$, i.e., for the π -flux chain along the armchair direction. However, in the armchair case, we numerically obtain a minigap within the in-gap band at the zone center and boundary ($k = \pi$). Figure 3(c) shows the gap Δ across zero energy at the zone center. For the chain along the zigzag direction, Δ exponentially decays as function of the interchain distance L_y , which signals gapless nature of the single chain. On the other hand, for the chain along the armchair direction, Δ saturates as a function of the interchain distance L_x , conveying that the minigap is not coming from size effects.

The π -flux may also be put on the hexagons of the second kind, for instance, by shifting the strings in Figs. 1(b) or 1(c) by the size of a single hexagon. The band structures for the π -flux chain threading the hexagons of the second kind are shown in the Supplemental Material [49]. It is shown that some states pop up (and down) from the bulk continuum to the gap for $|t_0| < |t_1|$, but there is no clear sign of zero-gap or near-zero-gap states. A consideration on the extreme limit of $t_0 = 0$ or $t_1 = 0$ gives some insights into the difference between threading the hexagons of the first and the second kinds and also the difference between $|t_0| > |t_1|$ and $|t_0| < |t_1|$. If we have $t_1 = 0$, the system is a set of isolated hexagons of the first kind. In such a case, it is easy to convince ourselves that the π -flux threading of those hexagons gives rise to zero-energy states, and nothing happens if the π -fluxes are misplaced. On the other hand, if we have $t_0 = 0$, the system is a set of dimers with no loops, making π -fluxes ineffective. Whether or not the zero-energy state in the extreme limit

survives in the interested parameter region is a nontrivial issue, and topology and symmetry come into play to help the zero-energy state survive, as we will see in the following.

Stability. The stability of the π -flux modes finds its origin in the existence of edge states and thus hangs directly together with the topological phase [19,20,32,33,35,50,51]. In fact, they provide for a direct bulk probe of the nontrivial symmetry-protected topology. As outlined in Ref. [32], this can be readily seen using a Volterra argument. Specifically, one can consider the effect of a π -flux by hypothetically cutting the system and then gluing back the two sides after the hopping elements over the segment that connects the boundary and defect core are multiplied with a π -phase, $e^{i\pi}$. When cutting the system results in edge states, gluing the sides together conventionally results in a mass term gapping the spectrum back to the original bulk situation. However, as the phases induce a minus sign for the hoppings on one side of the defect core, this mass term now switches sign. As a result, we obtain an effective Dirac system with changing mass term,

$$H_0 = v\sigma_3\mu_3 + m(x)\mu_1, \quad (1)$$

where v specifies the velocity, μ refers to the two edges of the Volterra cut, and σ parametrizes the pseudospin. Such Dirac theories with changing mass terms are well known to host localized soliton states at the mass domain wall, being the π -flux mode.

Our remaining task is to show the stability of the gapless edge mode supporting the description by Eq. (1). Here, we give two complementary explanations, one using a pseudo-time-reversal symmetry (TRS) and another using a mirror winding number. As for the former one, the system at hand is characterized by a $\mathbf{Z}_2$ classification, which is associated with a pseudo-time-reversal symmetry; see also the Supplemental Material [49]. In particular, time reversal, represented by complex conjugation $\mathcal{K}$, can be lifted to an antiunitary operation under C_n point group symmetries for $n = 4, 6$ [7]. The bands with complex values under the rotation operator (E representations), such as $|p_x\rangle$ and $|p_y\rangle$ states, come in pairs and induce a *two-dimensional real* representation due to the combination of both symmetries leading to degeneracies in the Brillouin zone. This also occurs in the present context, where doublets at the Γ point, arising by virtue of the sixfold symmetry, give rise to a nontrivial $\mathbf{Z}_2$ invariant. This argument only relies on doublets and has way broader applicability than our specific model; however, we note that this TRS comes from the crystal symmetry and only emerges in the effective model. In fact, the edge states can be gapped out by continuing away from the Γ -point, showing that the robustness of this symmetry is indeed not generally to be taken for granted.

Alternative, more rigorous, support for the gapless edge modes at zigzag edges comes from the combination of the chiral (sublattice) symmetry and the mirror symmetry, whose reflection plane is perpendicular to the zigzag edge [48,52]. The gaplessness comes from the degeneracy of the two zero modes having opposite chirality (sublattice polarization) and the opposite parity with respect to the reflection, guaranteed by nontrivial mirror winding numbers. In contrast to the pseudo-TRS-based argument, the mirror winding number is

completely robust, although the chiral symmetry is generically a strong constraint.

Finally, we turn to the gaplessness (minigap) of the midgap bands for the zigzag (armchair) π -flux chain, by focusing on the subspace spanned by the π -flux states. The above arguments suggest that the π -flux state inherits the properties of the edge states and the two bound states at a single π -flux have opposite chiralities (see Fig. 2). Then, within the effective model, we can take a basis such that the chiral operator γ becomes $\gamma = \sigma_3$, which gives us a chiral symmetric effective Hamiltonian

$$H(\tilde{k}) = h_1(\tilde{k})\sigma_1 + h_2(\tilde{k})\sigma_2, \quad (2)$$

where $\tilde{k} = k_x$ ($\tilde{k} = k_y$) for the zigzag (armchair) π -flux chain (see Fig. 1), referring to the x, y direction, whereas the value is set by the spacing of fluxes. For the zigzag π -flux chain, we also have the reflection symmetry $\sigma_3\hat{I}$, where $\hat{I}$ brings $\tilde{k}$ to $-\tilde{k}$, which commutes with γ at $\tilde{k} = 0$; see the Supplemental Material [49]. (Note that under the influence of the π -fluxes, the reflection symmetry actually means the spatial reflection associated with a proper gauge transformation.) This gives $h_{1,2}(-\tilde{k}) = -h_{1,2}(\tilde{k})$, and when we retain the nearest neighbor hoppings, the band structure will result in $E(\tilde{k}) \sim \pm|\sin\tilde{k}|$. On the other hand, for the armchair π -flux chain, the reflection symmetry becomes $\sigma_1\hat{I}$, which anticommutes with γ (see Supplemental Material [49]), giving us $h_1(-\tilde{k}) = h_1(\tilde{k})$ and $h_2(-\tilde{k}) = -h_2(\tilde{k})$. When we take only the leading contribution to $h_{1,2}(\tilde{k})$, the dispersion relation becomes $E(\tilde{k}) = \pm\sqrt{m^2 + \tilde{t}^2 \sin^2\tilde{k}}$. These arguments perfectly agree with the numerical results. As a side note, we mention that these considerations can also be phrased using a domain wall argument [35]. That is, one can readily formulate all symmetry-consistent couplings between the Volterra cuts and then project down to the subspace of the soliton solutions. These considerations then lead to the same effective Hamiltonian. Generalizing this description to account for the different symmetries involved for the zigzag and armchair edge then results in the same conclusions, while this setup also allows for the addition of other (TRS) symmetry-breaking terms. Similarly, we note that this analysis can also be applied in three dimensions (3D) [35]. That is, one can consider an array of flux lines, creating a sheet in the topological insulator. The extra dimension along the line then gives additional momentum, giving rise to anisotropic cones around the band nodes.

Perspective. Our demonstration suggests π -flux as a nice building block for designing various kinds of states. For instance, since the π -flux state is localized, simply making the distance between the threaded hexagons away results in flattened bands. Figure 4 shows such examples, i.e., we observe smaller total band width of the in-gap states in the case of larger distance between the threaded hexagons. For the chains along the armchair direction, the minigap is also reduced, which has also been detected in Fig. 3(c). The advantage of using π -fluxes as building blocks is that the existence of zero-energy states are guaranteed by *topological protection*. In addition, in the same modulated honeycomb lattice model, edge states, or interface states at the boundary between two regions with $|t_0| > |t_1|$ and $|t_0| < |t_1|$ have been investigated. As we have noted, the interface-edge states and

FIG. 4. Flatter in-gap bands for larger π -flux spacing. Panels (a) and (b) show $\{L_x, L_y\} = \{6\sqrt{3}a_0, 36a_0\}$ and $\{L_x, L_y\} = \{12\sqrt{3}a_0, 9a_0\}$, respectively. For panel (a), π -flux threaded hexagons essentially align in the zigzag direction, while for panel (b), they align in the armchair direction.

the π -flux states share the same origin, and thus there is no need for fine-tuning to have them in the same gap. Hence, it is an interesting future problem to look for new states or phenomena caused by interplay between edge-interface states and π -flux states.

Experimental implementation. Obviously, the key ingredient to realize π -flux is feasibility of the sign flip of the hopping. In some artificial systems, schemes to change the sign of the coupling have already been proposed. For instance, Ref. [53] proposes a mechanical system made of disks and springs, and there “normal” and “reversed” springs leading to opposite signs of couplings are introduced. Sometimes, spring-based discrete systems are effectively or essentially realized in continuous elastic media with springs being substituted by beams. Mapping a discrete model to a continuous model is a nontrivial task, but once the mapping is established, current 3D printing techniques will enable us to fabricate designed elastic media [54]. Another promising scheme is to use LC circuits. The authors of Ref. [55] propose and experimentally implement clever wiring between elements to integrate 0-phase and π -phase hoppings into a single system to show Berry curvature and Fermi arcs.

In terms of the implementation, it is worth noting another route: Controlling site potential can induce the sign flip of the

effective hopping, as roughly sketched as follows. Let us focus on two sites across which we want to induce hopping. Then, instead of directly connecting them, we put an extra intermediate site connected to the both of them by hopping t . When the difference of the site potentials for the intermediate and the focused sites ΔE is large, the second-order perturbation gives an effective hopping between the focused sites $t^2/\Delta E$, which means that the sign of the effective hopping depends on the sign of ΔE .

Conclusion and discussion. We have shown that π -flux modes, characterizing topological band insulators, can be naturally realized in artificial materials. Given the *direct* implementability of artificial materials, this creates a promising scene to study π -flux modes as well as the highly tuneable bands that arise from their hybridization. More generically, these modes can be used as building blocks, opening up the door to an experimentally viable setting in which numerous models incorporating fluxes (vortex lattices, lattice gauge theories etc.) and the associated effective (field) theories can be brought to life.

We note that in contrast to electron systems, such bosonic setups do not have a natural filling, constraining the possibilities of anomalies that also arise due to an interplay with the edge states of the parent model [35]. However, the midgap modes still can be viewed as extra conducting channels, which will have graphene-like signatures (or, in fact, half-graphene-like signatures due to the absence of a valley degree of freedom). Indeed, as alluded to above, an interesting direction will be to study the interaction with edge states, considering extended flux lattices connecting edges. This similarly applies to studying junctions of flux lattices in the bulk where the modes can form new transporting architectures. Finally, we also intend to study dense flux lattices in which the bound modes can hybridize into novel band structures [56] that can have (higher) Chern numbers depending on the coordination of this flux lattice. Motivated by these results and possible routes, we hope that our work will inspire a range of future pursuits.

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