Editors' Suggestion

Fragile Topology and Wannier Obstructions

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Topological phases, such as Chern insulators, are defined in terms of additive indices that are stable against the addition of trivial degrees of freedom. Such topology presents an obstruction to any Wannier representation, namely, the representation of the electronic states in terms of symmetric, exponentially localized Wannier functions. Here, we address the converse question: Do obstructions to Wannier representation imply stable band topology? We answer this in the negative, pointing out that some bands can also display a distinct type of "fragile topology." Bands with fragile topology do not admit any Wannier representation by themselves, but such a representation becomes possible once certain additional trivial degrees of freedom are supplied. We construct a physical model of fragile topology on the honeycomb lattice that also helps resolve a recent puzzle in band theory. This model provides a counterexample to the assumption that splitting of an "elementary band representation" introduced in [B. Bradlyn et al., Topological quantum chemistry, Nature (London) 547, 298 (2017)] leads to bands that are individually topological. Instead, half of the split bands of our model realize a trivial band with exponentially localized symmetric Wannier functions, whereas the second half possess fragile topology. Our work highlights an important and previously overlooked connection between band structure and Wannier functions, and is expected to have far-reaching consequences given the central role played by Wannier functions in the modeling of real materials.

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Introduction.—In recent years, there has been rapid development of our understanding of topological phases. One important area of activity has been to classify all possible, distinct gapped phases by relating them to appropriate mathematical classification schemes. For noninteracting fermions in the presence of only internal symmetries (such as time-reversal symmetry), a classification of states with a bulk energy gap has been obtained using K theory [1]. Conceptually, states with nontrivial topology are readily identified from their gapless edge states, while the trivial state has a boundary that can be gapped without breaking symmetry [2–5]. An important feature of such classification schemes is the notion of stability, that is, the requirement that a topological phase is robust to the addition of trivial, weakly coupled degrees of freedom (d.o.f.) [1–6].

For crystalline systems, however, new physical complications arise. First, the presence of crystalline symmetries can protect new kinds of topological phases [7,8], which are captured by extensions of the K-theory classification scheme to the case of crystalline symmetries [9–13]. Unlike phases protected solely by internal symmetries, phases protected by crystalline symmetries may not possess any gapless surface states, as it may not be possible to find a surface that respects all the protecting symmetries. Second, there are cases where, despite a clear bulk distinction between two phases, it is physically unclear which one is to be labeled trivial and which topological; rather, what is well defined is *relative* topology, which concerns whether or not two systems are distinct phases separated by a bulk gap closing when symmetries are preserved throughout the deformation. For instance, spatial symmetries can lead to mutually distinct product states [14]. Specializing the discussion to electronic phases, product states correspond to strict atomic insulators, defined as the full filling of a set of strictly localized orbitals. Their insulating nature can be explained even if one models electrons as classical particles trapped in periodic potential wells [15]. Such phases do not have any symmetry-protected quantum entanglement, and therefore we label all atomic insulators as trivial [15–19].

In contrast, a weakly correlated crystal is insulating whenever the electronic energy bands, a concept defined in the momentum space, are gapped at the Fermi energy. This is more general than the real-space, atomic picture we described, and a topological band insulator arises precisely when there is an obstruction in describing the system using any atomic picture [15–19].

The contrast between the momentum- and real-space descriptions of a band insulator is closely related to the notion of Wannier functions, which is a generalization of atomic orbitals. Consider a group of isolated bands. Following the definitions above, we say they are trivial if and only if they can be represented in terms of exponentially localized Wannier functions that preserve

all symmetries. For brevity, we refer to this property as "Wannier-representable," with the understanding that the Wannier functions involved are exponentially localized and respect all symmetries. In this terminology, when the set of valence bands of a system is Wannier representable, the ground state is a trivial atomic insulator; conversely, a set of topological bands will be obstructed from any Wannier representation.

It is important to connect our discussion to the more conventional notion of (symmetry-protected) topological indices of band structures. Familiar topological phases characterized by, say, a nontrivial Chern number automatically feature a Wannier obstruction [16]. More generally, such Wannier obstructions are present for any band structure with a nontrivial K-theoretic topological index [1,9–13], provided that the index is not describing the mutual topology between atomic insulators [11,18].

However, the converse need not be true; i.e., there could be examples of bands which are not Wannier representable, even when all the K-theoretic indices are compatible with a trivial phase. This possibility originates from a strong sense of robustness (known technically as "stable equivalence") demanded in the K-theory-based classification of band insulators, which is more stringent than what the physical problem calls for [9]. We present a concrete example in this work, where we demonstrate that a set of Wannier-obstructed bands can be explicitly trivialized simply by the presence of an additional atomic insulator. The band topology in the Wannier-obstructed bands is therefore weaker than that of familiar, stable topological phases captured within K theory, and we refer to it as fragile topology.

We now highlight some applications of the fragile topology concept, both to the conceptual as well as to the practical aspects of band structures. First, we stress that this concept has important implications for the modeling of correlated materials. There, one seeks to capture the bands of interest by a tight-binding model into which one incorporates electron-electron interactions. The tight-binding model itself is obtained from the Wannier functions; hence if the relevant bands possess a fragile topology, the resulting Wannier obstruction implies that this canonical procedure will fail at the first step. It can be remedied only by incorporating additional carefully selected orbitals. That this is not an academic issue was emphasized in recent discussions [20–23] of the band structure of twisted bilayer graphene (TBG), where ground-breaking experiments have discovered a correlated insulator and a superconductor [24–26]. It was pointed out in Ref. [20] that the relevant bands in TBG suffer from a Wannier obstruction if all symmetries are included, despite the absence of any known stable topological phase in this symmetry setting.

Second, we point out that a proper understanding of fragile topology is crucial for utilizing the recent proposal in Refs. [19,27,28], which asserted that an exhaustive comparison of symmetry representations in momentum space and real space will lead to an efficient diagnosis of topological materials. We clarify that, if the supposedly topological filled bands feature only fragile but not stable topology, the actual topological properties of the materials could be trivialized merely by the presence of filled bands corresponding to closed-shell electrons. Finally, we note that although topological properties of the (non-Abelian) Berry phase of band structures are commonly taken as a defining feature of topological crystalline phases [29–33], they imply only a Wannier obstruction and not necessarily stable topology.

A honeycomb lattice model.—We begin by describing our construction of a four-band model on the honeycomb lattice, which splits into conduction and valence bands, each consisting of two bands, separated by a band gap. We later show that the valence bands of our model are trivial, whereas the conduction bands feature fragile topology.

Consider a honeycomb lattice with the origin placed at the center of a hexagon and a p_z orbital localized to each of the sites. We assume the system is symmetric under time-reversal but not spin rotations, which is a natural setting in the presence of strong spin-orbit coupling. We assume the spatial symmetries of the wallpaper group No. 17 (SG No. 183), which describes the symmetries of the two-dimensional system placed on a symmetry-matched substrate [19,27,34,35]. We denote this wallpaper group by $\mathcal{G}$, and let $\mathcal{P}$ be its point group ($6mm$). $\mathcal{P}$ is generated by a sixfold rotation about the hexagon center and a mirror along a line passing through a nearest-neighbor bond. We always assume periodic boundary conditions.

Our goal is to construct a model with fragile topology. To this end, one should first rule out the presence of stable topology. In our context, such a model can be constructed as follows: Starting with the Kane-Mele model [34,35] with inversion symmetry [Fig. 1(a)], which has a nontrivial $\mathbb{Z}_2$ quantum spin Hall index, we add additional terms to induce a band inversion at Γ [Fig. 1(b)]. This trivializes the $\mathbb{Z}_2$ quantum spin Hall index. However, as the inversion symmetry combines with a two-dimensional C_2 rotation into a mirror in the plane parallel to the system, one can only conclude that the system has an even mirror Chern number [7]. The last step, therefore, is to break inversion symmetry, and hence the mentioned mirror. This gives a model without any known topological invariant.

We now construct our model $\hat{H}_0$ explicitly. This is achieved by first specifying a collection of time-reversal symmetric bonds, and then symmetrizing by summing over all the g-related bonds for $g \in \mathcal{G}$. For the bond $i(=1,2,\ldots,5)$ represented by an arrow going from site $\boldsymbol{x}$ to $\boldsymbol{y}$ [Fig. 1(c)], we define

$$\hat{h}^{(i)} \equiv \sum_{\alpha,\beta=\uparrow,\downarrow} \hat{c}^{\dagger}_{\boldsymbol{y},\alpha}\left(\tau^{(i)}\sigma_0 + i\boldsymbol{\lambda}^{(i)}\cdot\boldsymbol{\sigma}\right)_{\alpha\beta}\hat{c}_{\boldsymbol{x},\beta}, \tag{1}$$

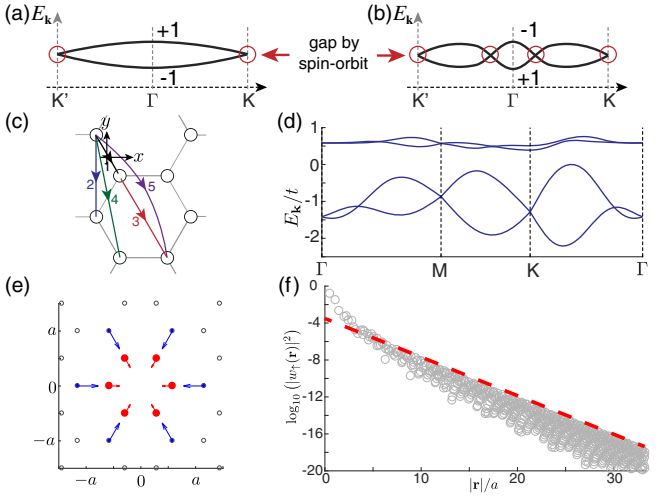

FIG. 1. Model for fragile topology. [(a) and (b)] Construction of model with fragile topology. (a) The nontrivial $\mathbb{Z}_2$ index of the Kane-Mele model [34,35] can be diagnosed from the inversion eigenvalues of the bands [36], as we labeled for Γ. The role of spin-orbit coupling is to open a gap. (b) A further band inversion at Γ trivializes the $\mathbb{Z}_2$ index. (c) Terms in the Hamiltonian $\hat{H}_0$. (d) Band structure of the honeycomb Hamiltonian, with a clear band gap at a filling of two electrons per unit cell. (e) A symmetric Wannier function $w_\uparrow(\boldsymbol{r})$ centered at the origin. a denotes the lattice constant. The other Wannier function, also centered at the origin, can be obtained by applying time reversal. We visualize it by an arrow and a circle attached to every site at which $|w_\uparrow(\boldsymbol{r})|^2 > 0.3 \times 10^{-2}$. Red (blue) filled circles indicates that, locally, the spin is tilting up (down), and their sizes represent the relative weights of the Wannier function. The arrow shows the in-plane component of the spin. (f) $|w_\uparrow(\boldsymbol{r})|^2$ decays exponentially at large distances (red dashed line).

where $\hat{c}_{\boldsymbol{x},\alpha}$ and $\hat{c}_{\boldsymbol{y},\alpha}$ respectively denote the fermion annihilation operators for a spin-α electron localized at sites $\boldsymbol{x}$ and $\boldsymbol{y}$, and σ_j's denote the standard Pauli matrices [37]. Here, $(\tau^{(i)}, \lambda_1^{(i)}, \lambda_2^{(i)}, \lambda_3^{(i)})$ are four dimensionless real parameters defining the electron hopping along bond i. Their chosen numerical values are tabulated in Supplemental Material (SM) [38]. Note that we have optimized our model for achieving a more sizable band gap, which leads to longer range hopping (up to fifth-nearest neighbors). Nonetheless, we stress that only finite-range hoppings are considered, and so long as both the band gap and symmetries are maintained the general features we describe below persist against perturbations.

The honeycomb model is then defined by

$$\hat{H}_0 = \frac{t}{|\mathcal{P}|} \sum_{i=1}^{5} \sum_{g \in \mathcal{G}} \hat{g}\, \hat{h}^{(i)} \hat{g}^{-1} + \text{H.c.}, \tag{2}$$

where $|\mathcal{P}| = 12$, and $t > 0$ is an overall energy scale. As shown in Fig. 1(d), a gap at half filling is found at all high-symmetry momenta. Considering also the interior of the Brillouin zone (BZ), one finds a band gap [39] of $0.39t$. For comparison, the valence bandwidth is $\sim 2t$.

Our next goal is to analyze the band topology present in $\hat{H}_0$. In particular, we first establish that the valence bands are trivial.

Trivial valence bands.—As a first check, we construct symmetric Wannier functions of the valence bands [40,41]. No obstruction was encountered in this process (SM), and the results are visualized in Fig. 1(e). The weight of a Wannier function as a function of r, the distance away from its charge center (which sits at the center of a hexagon), is shown in Fig. 1(f). The weight decays exponentially as $r \to \infty$, decaying by 4 orders of magnitude in ten lattice constants. This implies the valence bands of $\hat{H}_0$ admit symmetric, exponentially localized Wannier functions, and therefore the corresponding band insulator is trivial. In SM, we also provide an alternative proof of its triviality through an adiabatic, symmetric deformation to an explicit atomic limit.

Nontrivial conduction bands.—Since the conduction bands of $\hat{H}_0$ combine with the valence bands to form an atomic insulator (namely, the p_z orbitals localized to the honeycomb sites), the triviality of the valence bands rules out any stable topology in the conduction bands. However, based solely on the symmetry representations of the conduction bands (available, e.g., on the Bilbao crystallographic server [27]), one can see that the conduction bands cannot be Wannier representable. This is because any atomic insulator at a filling of two electrons per unit cell must have the electrons localized to the triangular lattice sites, and one can check that no such atomic insulator possesses the same set of symmetry representations as the conduction bands at all momenta [19,27,28]. As symmetry representations are bulk quantities which cannot be modified without a band-gap closing, they serve as a nontrivial topological invariant for the conduction bands. Note that a representation-based invariant is as robust as that arising from more involved objects, say from the Wilson loops [29–33].

It is conceptually revealing to connect our present observations to the discussions in Ref. [18], which discussed how symmetry eigenvalues can inform band topology in two different ways. The first is embodied in the notion of "symmetry-based indicators of band topology," which is concerned with stable topology. The second diagnosis is more subtle, and is tied to the distinction between the physical stacking and the formal addition of atomic insulators, where a (formal) subtraction between atomic insulators is allowed only in the latter but not the former. By formal subtraction, we mean the following: let $\mathcal{A}$, $\mathcal{V}$, and $\mathcal{C}$ be gapped bands such that $\mathcal{A}$ can be viewed as arising from stacking the bands $\mathcal{V}$ and $\mathcal{C}$, i.e., $\mathcal{A} = \mathcal{V} \oplus \mathcal{C}$. Then we can formally identify $\mathcal{C}$ as the difference between $\mathcal{A}$ and V. Crucially, even when both $\mathcal{A}$ and $\mathcal{V}$ above are atomic insulators, $\mathcal{C}$ may not admit a Wannier

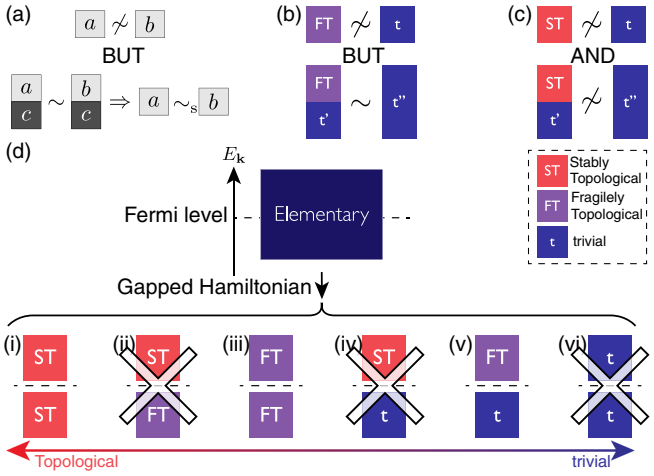

FIG. 2. Fragile topology and decomposable elementary band representations. (a) In a K-theory-based classification [1,9–13], it could be that two band insulators a and b are not smoothly connected, but the obstruction is resolved once we append to both sides an additional set of bands c. We say a and b are stably equivalent, denoted by $a \sim_s b$. (b) Using similar ideas, we introduce the notion of fragile topology. We say a set of bands possesses fragile topology if there is a topological obstruction in deforming it to any trivial (atomic) limit, but the obstruction is resolved once we allow for the introduction of additional trivial d.o.f. (c) In contrast, bands with stable topology remain nontrivial upon the stacking of any trivial bands. (d) Up to an overall sign change of the tight-binding Hamiltonian, there are generally six distinct splitting patterns for a decomposable elementary band representation. Three cases are ruled out by definitions, indicated by crosses. Our model $\hat{H}_0$ shows that case (v), the only splitting pattern with trivial valence bands, is possible.

representation. Such is the case for the conduction bands ($\mathcal{C}$) of $\hat{H}_0$, which can be viewed as subtracting the valence bands ($\mathcal{V}$), an atomic insulator with electrons localized to the triangular sites, from the atomic insulator formed by full filling of the honeycomb sites ($\mathcal{A}$). In fact, such systems are prime candidates for fragile topology, since by definition the symmetry representations do not indicate any necessary stable topology. We also note that some "filling-enforced quantum band insulators" discussed in Ref. [15] also sit in this class [18], and therefore they might be early examples of fragile topology.

Fragile topology and band representations.—Having established the existence of fragile topology in the conduction bands of the concrete model $\hat{H}_0$, we discuss its general implications. As we have alluded to, the key difference between stable and fragile topology descends from the notion of stable equivalence in K theory [Fig. 2(a)]. It is instructive to provide a more precise definition. Consider an isolated set of bands, and we ask if it can be represented in terms of exponentially localized Wannier functions that respect all symmetries. If this is possible, the set of bands is trivial. If this fails, we can further ask: can we add to this set another set of trivial bands, derived from an atomic insulator, and then obtain localized Wannier functions? If yes, our original set only possesses fragile topology [Figs. 2(b) and 2(c)]. By this definition, the valence bands of our model are trivial, and the conduction bands possess fragile topology. We also provide a more physical perspective on the preceding discussion in SM.

Next, we connect the phenomenology of fragile topology to a recent proposal [19,27,28] that the theory of band representations, developed by Bacry *et al.* [42–45], can lead to a general classification of topological band insulators. (Please see SM for a brief introduction to the notion of band representations.) A key idea in this proposal is that of an "elementary band representation" (EBR) [42–45], which has the defining feature that, if it splits in momentum space into disconnected (i.e., separated by a band gap) conduction and valence bands, then the two sets of bands cannot be simultaneously trivial [19,27,28].

In fact, as is discussed in depth in Refs. [19,27], the tight-binding d.o.f. specified in $\hat{H}_0$ correspond to an EBR, and therefore $\hat{H}_0$ serves as a concrete model realization of the splitting pattern "EBR = trivial $\oplus$ fragilely topological." Given the ground state of $\hat{H}_0$ is an atomic insulator, we conclude that the splitting of an EBR does not generally imply nontrivial band topology in an insulator.

Discussion.—We emphasize that while fragile topology may be reminiscent of the "Hopf insulator" [46,47], they are sharply distinct concepts. Without adding additional symmetries, the Hopf insulator is only topological in a half-filled two-band model [48], and is unstable even against the introduction of high-energy, unoccupied d.o.f. Therefore, topology of the Hopf insulator variety is not expected to be relevant to electronic band structures in materials, where such high-energy bands are inevitably present. In contrast, fragile topology remains well defined in this setting, and is only trivialized by adding fully filled atomic bands below the Fermi level. The distinction between adding orbitals above and below the Fermi energy is important because only the latter necessitates a modification of the many-body wave function. In addition, unlike the Hopf insulator, the notion of fragile topology does not rely on the nontriviality of any special map between spaces, and is ultimately defined via the symmetry protection of certain patterns of quantum entanglement in the ground state wave function. It is expected to arise whenever the spatial symmetries are rich enough, for systems with or without spin-orbit coupling and/or time-reversal invariance, in both two and three dimensions.

Our model also proves that the splitting of an EBR, discussed in Refs. [19,27,28], does not necessarily imply a topological band insulator, and for a reliable diagnosis one must further corroborate analysis using symmetry eigenvalues [18,19,27,28,49–53] or, more generally, wave-function-based topological invariants. We note that the range of physical signatures that a fragile topological phase

can exhibit is expected to be restricted by the fact that it can be trivialized by stacking with an atomic insulator. For instance, fragile topological phases are not expected to host protected surface states, for their bulk topology can be trivialized simply by the addition of atomic insulators without any surface signatures. This also suggests fragile topology is not expected when only internal symmetries are present, since one can always find a surface which preserves all internal symmetries. We leave the analysis of their physical signatures and general diagnosis to future works.

In closing, we emphasize that the notion of fragile topology is important in the modeling of electronic systems, given the central role played by Wannier functions in the well-established methods. Moreover, fragile topology is not a mere mathematical possibility, but arises in realistic models and potentially even in real materials, like small-angle twisted bilayer graphene [20–23].

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[37] Here, we take spin-up to be aligned with the crystallographic z axis, which is normal to the two-dimensional system.
[38] See Supplemental Material http://link.aps.org/supplemental/10.1103/PhysRevLett.121.126402 for for notes on further details of the model, a deformation to an explicit atomic limit, construction of Wannier functions, a more physical view on fragile topology, relation between K-theory and fragile topology, and the notion of band representations.
[39] Defined in this work as the difference between the bottom of the conduction band and the top of the valence bands, which lower bounds the "direct band gap" definition common in the study of topological band insulators.
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