In a remarkable pair of papers, Kane and Mele [1, 2] proposed a $\mathbb{Z}_2$ topological invariant of time-reversal-invariant insulators in two dimensions, showed that the nontrivial “topological insulator” phase created by spin-orbit coupling has an intrinsic spin Hall effect distinct from earlier proposals [3, 4], and argued that graphene is a viable system in which to observe this effect. (Here $\mathbb{Z}_2 \equiv \mathbb{Z}/2\mathbb{Z}$ is the cyclic group of two elements.) A direct and experimentally relevant characterization of the invariant was given in terms of edge states at the boundary of a 2D insulator: the topological insulator has an odd number of Kramers pairs of edge modes, while the ordinary insulator has an even number. Two explanations for the invariant as a property of the bulk band structure with spin-orbit coupling were also given.

We first show that time-reversal-invariant ($T$-invariant) 2D insulators have multiple $\mathbb{Z}_2$ invariants that are directly analogous to the band $\mathbb{Z}_2$ invariants of a single bulk $\mathbb{Z}_2$ invariant, which do not follow the standard homotopy paradigm of most topological invariants in condensed matter physics, and whose connection to the IQHE is opaque: for the case of an occupied pair of bands relevant to graphene, the $\mathbb{Z}_2$ invariant was explained either by invoking K-theory (recently used to classify Fermi surfaces [5]) or by counting zeroes or zero regions of a certain matrix Pfaffian.

The $\mathbb{Z}_2$ invariant is first rederived for the simplest case (two occupied bands related by time-reversal symmetry) using basic homotopy theory to establish its connection to the usual Chern number or TKNN integer [6] of $T$-invariant systems. There is a connection between its absence with inversion symmetry and previous work on topological invariants of $T$-invariant Fermi systems [7].

We then obtain results for multiple occupied bands: there are multiple $\mathbb{Z}_2$ invariants in such systems, and perhaps most interestingly, four invariants per band in 3D. In 2D, the significance of these invariants in physical systems is straightforward: just as two IQHE states with the same sum of Chern numbers for occupied bands are adiabatically connected, two $T$-invariant band insulators are adiabatically connected if and only if they have the same $\mathbb{Z}_2$ sum of individual $\mathbb{Z}_2$ invariants.

The approach in this paper can be outlined as follows. The basic objects of homotopy theory are the homotopy groups $\pi_n(M)$ that describe equivalence classes under smooth deformations of mappings from the sphere $S^n$ to a manifold $M$. A band structure can be thought of as a map from the Brillouin zone (a torus rather than a sphere) to the space of Bloch Hamiltonians, assuming that the Hilbert space is the same for all points in the Brillouin zone. The $T$ symmetry means that the effective Brillouin zone (EBZ), a set of points for which the Bloch Hamiltonians can be specified independently, is nearly a sphere: we consider “contractions” that extend a mapping from the EBZ to one from the sphere.

A given mapping from the EBZ has an infinite set of topologically inequivalent contractions in this sense. We consider a mapping from the EBZ together with the set of all of its contractions, which is invariant under smooth deformations of the original mapping. There are then exactly two equivalence classes, for the case of two occupied bands connected by $T$, which correspond to the ordinary insulator and the topological insulator. In this simplest case, an ordinary (topological) insulator becomes the equivalence class of all mappings from the sphere with even (odd) Chern numbers. This construction requires only standard homotopy results, makes no assumptions about the details of the band structure or the existence of additional commuting operators such as spin, and generalizes directly to multiple bands and higher dimensions.

For 2D $T$-breaking systems, in a nondegenerate band
where the second formula indicates Hamiltonians as upon the same Hilbert space. Denoting the space of such operators, which are assumed to be nondegenerate and act is by considering mappings of the torus to Bloch Hamiltonians, which are assumed to be nondegenerate and act upon the same Hilbert space. Denoting the space of such Hamiltonians as $M$, the existence of the TKNN integers follows from the first two homotopy groups
\[ \pi_1(M) = 0, \pi_2(M) = \mathbb{Z}^{n-1}, \]
where the second formula indicates $n - 1$ independent integer-valued invariants because the invariants sum to zero. There are a number of ways to obtain the TKNN integers, e.g., as an integral over the magnetic Brillouin zone (a torus) of the Berry flux, using the explicit wavefunction $|\psi_i\rangle$ for band $i$, or as an integral using the projection operator $\mathbb{P}$
\[ n_i = \frac{i}{2\pi} \int_{BZ} \text{Tr}(dP_i P_i dP_i), \quad P_i = |\psi_i\rangle\langle\psi_i|. \] (1)
Here $dP_i = dx\partial_x P_i + dy\partial_y P_i$ and $dx dy = -dy dx$. A powerful way to understand these integer invariants is by considering mappings of the torus to Bloch Hamiltonians, which are assumed to be nondegenerate and act upon the same Hilbert space. Denoting the space of such Hamiltonians by $C$, the two-fold degeneracy required by $H$ is represented by an antiunitary operator $\Theta$ in the finite cyclic group $\mathbb{Z}_2$. For a pair of bands $i, j$ that are possibly degenerate with each other but with no other bands, there is a single integer-valued invariant $\mathbb{P}$ obtained by replacing $P_i$ in $\mathbb{P}$ with $P_{ij} = P_i + P_j$.

FIG. 1: The topology of the effective Brillouin zone (EBZ): if the original Brillouin zone is the torus in (a), then $T$-invariance reduces the independent degrees of freedom to live on the manifold in (b). Points on the boundary circles that are connected by horizontal lines are conjugate under $T$; the points $\Gamma, A, B, C$ are self-conjugate, and their Bloch Hamiltonians are therefore in the even subspace $Q$.

Now consider consequences of invariance under the time-reversal operator $T$. For fermions, $T^2 = -1$ and $T$ is represented by an antunitary operator $\Theta$ in the Hilbert space of Bloch Hamiltonians. Time-reversal connects both pairs of points in the Brillouin zone $(k, -k)$ and the associated Bloch Hamiltonians:
\[ H(-k) = \Theta H(k)\Theta^{-1}. \] (3)

Fig. 1 shows the original toroidal Brillouin zone and the EBZ: specifying the Hamiltonians for all points on the EBZ determines them everywhere. The Bloch Hamiltonians can be specified independently except at the boundaries, where points are related by $T$. Clearly points at which $k = -k$, such as $\Gamma, A, B, C$ in Fig. 1, are special: at these points the Bloch Hamiltonian commutes with $\Theta$. This “even” subspace in the language of Ref. 1 has a natural interpretation as the set of symplectic or quaternionic Hamiltonians: we denote this subspace, with the additional assumption of no degeneracies other the two-fold degeneracies required by $T$, as $Q$. $T$-invariance requires an even number of bands $2n$.

In general, a $T$-invariant system need not have Bloch Hamiltonians in $Q$ except at these special points as long as inversion symmetry is broken, so that $H(k) \neq H(-k)$. At first glance, there is no obvious topological invariant for a degenerate band with time-reversal symmetry, because the Chern number for the whole Brillouin zone vanishes. It is simplest to see this for the projection operator $P_i$ corresponding to a single nondegenerate band: using an explicit representation $P_i = |\psi_i\rangle\langle\psi_i|,
\[ n_i = \frac{i}{2\pi} \int_{BZ} \text{Tr}(dP_i P_i dP_i) \]
\[ = \frac{1}{2\pi} \text{Im} \int \left[ (\partial_x \psi_i | \partial_y \psi_i) + (\partial_y \Theta \psi_i | \partial_x \Theta \psi_i) \right] \]
\[ = \frac{1}{2\pi} \text{Im} \int \left[ (\partial_x \psi_i | \partial_y \psi_i) + (\partial_y \psi_i | \partial_x \psi_i) \right] = 0. \] (4)
A similar argument applies for two possibly degenerate bands, but there is nevertheless a topological invariant, and in general multiple topological invariants.

As a quick example of homotopy arguments, suppose that inversion symmetry is unbroken, which implies that the Bloch Hamiltonians are everywhere in $Q$. Any mapping of the torus $T^2$ to $Q$ with the condition that points $k$ and $-k$ go to the same point is determined by its behavior on one point from each $(k, -k)$ pair, and the EBZ under this condition is topologically identical to a sphere (stitching $T$-conjugate points together in Fig. 1b): the classes of such mappings are given by $\mathbb{Z} \pi_2(Q) = 0$. Hence there is no homotopy invariant for 2D band structures with both $T$ and inversion symmetry, although $\pi_4(Q) \neq 0$ and higher-dimensional invariants can exist.

Now consider possible invariants without inversion symmetry. We seek to classify mappings from $T^2$ to the space of Hamiltonians $C$ that have at most two-fold degeneracies within a pair of $T$-related bands and behave under $\Theta$ as specified above. Such a mapping is determined by a mapping from the EBZ, i.e., a mapping from the cylinder $C$ to $C$ with certain conditions on the two circular boundaries reflecting time-reversal. The image of a boundary point must be the $\Theta$ conjugate of the image of the point on the same boundary related by $k \leftrightarrow -k$.

If the same Hamiltonian occurred at all points on the boundary, then the topology of the cylinder becomes that
of the sphere, and the degenerate Chern numbers [8] are integer-valued invariants for mappings from the sphere to \( \mathcal{C} \) that give one integer for each possibly degenerate pair since \( \pi_2(\mathcal{C}) = \mathbb{Z}^{n-1} \). For the simplest case of two occupied possibly degenerate bands, the invariant combination reduces to \( n_1 + n_2 \) if the bands are nondegenerate and hence have separate Chern numbers \( n_1 \) and \( n_2 \).

We show first for the simplest case of one pair of bands that any mapping from \( \mathcal{C} \) to \( \mathcal{C} \), even if the elements at a boundary are not all the same, can be smoothly deformed (“contracted”) to one in which the boundary elements are identical to an arbitrary reference element \( Q_0 \in \mathcal{Q} \) (Fig. 2a); the resulting map from the sphere has a well-defined Chern number. It is required that at each stage of the contraction, the boundary has the same conjugacy of points under \( T \) as in the original boundary. This guarantees that two maps from the EBZ that can be contracted to maps from the sphere with the same Chern number are homotopic (deformable to each other).

Then it is shown that different contractions differ by an arbitrary even Chern number, so that there are only two possibilities for homotopy (deformable to each other). The fact that different contractions differ by an even Chern number is less trivial and gives an unexpected picture of how the \( \mathbb{Z}_2 \) invariant arises: as an embedding of one \( \mathbb{Z} \) homotopy group in another. Whether a band is “odd” or “even” is directly computable by using any contraction to define the Chern number integral.

A contraction in the sense above gives a smooth mapping from a cylinder to \( \mathcal{C} \), \( f(\theta, \lambda) \), \( 0 \leq \lambda \leq 1 \) such that for each \( \lambda \), \( f(\theta, \lambda) \) and \( f(2\pi - \theta, \lambda) \) are \( T \) conjugates (which implies that \( f(0, \lambda) \) and \( f(\pi, \lambda) \) are in \( \mathcal{Q} \)). Now \( f(\theta, 0) \) should agree with the initial specification of Bloch Hamiltonians, while \( f(\theta, 1) = Q_0 \) is constant. If both boundaries are contracted, the resulting sphere has a well-defined Chern number for each pair of bands.

In fact, many topologically inequivalent contractions exist, and these different contractions are responsible for reducing the integer-valued invariants on the sphere to \( \mathbb{Z}_2 \) invariants on the EBZ. Let \( f_1 \) and \( f_2 \) be two different contractions. Then define a mapping \( g(\theta, \lambda) \), which by composition changes from contraction \( f_1 \) to \( f_2 \) (Fig. 2b):

\[
g(\theta, \lambda) = \begin{cases} f_1(\theta, 1 - 2\lambda) & \text{if } 0 \leq \lambda < 1/2 \\ f_2(\theta, 2\lambda - 1) & \text{if } 1/2 \leq \lambda \leq 1. \end{cases} \tag{5}
\]

Although the domain of the mapping \( g \) is topologically a sphere because the circles at both ends go to the same point, \( g \) differs in its \( T \) symmetry from the contracted half of the Brillouin zone, which in its interior has no \( T \) symmetry relating different values of \( \theta \). Let the cylinder in the definition of \( g \) have coordinates \( \theta \in [0, 2\pi) \), \( \lambda \in [0, 1] \); then points \((\theta, \lambda)\) and \((2\pi - \theta, \lambda)\) are \( T \)-conjugate.

It follows that \( g \) has arbitrary even Chern numbers, and the change in the Chern numbers of \( n_B \) induced by changing from contraction \( f_1 \) to contraction \( f_2 \) is

\[
\Delta n_B^i = 2n_B^i, \tag{6}
\]

where \( i \) indexes band pairs. This can be verified in two steps: map the equator of the sphere \( S \) to the constant element \( E_0 \), which is possible since \( \pi_1(\mathcal{Q}) = 0 \) and topologically unique since \( \pi_2(\mathcal{Q}) = 0 \), then note that each hemisphere has a well-defined Chern number and that the Chern numbers of the two hemispheres are equal, rather than opposite as in the case of the original Brillouin zone. The reason for this equality can be understood easily in the cylindrical coordinates above, where the equator is at \( \theta = \pi \) and \( \theta = 0 \). The identification under \( T \) of \( \theta \) and \( 2\pi - \theta \) means that \( d\theta \) changes sign between a point and its time-reversal conjugate, but \( d\lambda \) does not, giving an additional change of sign in equation (4).

The same topological argument applies to \( n \) pairs of bands. Since there is one integer invariant for each such pair with a zero sum rule, there is one \( \mathbb{Z}_2 \) invariant for each pair, with an even number of “odd” band pairs.

We now give the generalization to three-dimensional Brillouin zones, where there are significant differences between \( \mathbb{Z}_2 \) invariants and the 3D integer-valued TKNN invariants [4, 8]: there are four independent \( \mathbb{Z}_2 \) invariants per pair of bands, even though there are only 3 Chern numbers for a pair of degenerate bands. An alternate way to obtain the 2D result, which is more useful for 3D, is by considering contractions to a torus, rather than a sphere. The set of mappings from the Brillouin zone \( T^3 \)
Chern numbers, one for the $xz$ topic as maps to have the same Chern number (zero) and thus are homogeneous while the other is odd because the boundary slices $Z^T$ that reduce the degrees of freedom to the 2D BZ. The reduction of an original 3D EBZ to the torus is invariant in 3D. Suppose that the Brillouin zone $C^T$ planes in $xz$ and $xy$ constraint means that the $Z^T$ planes: it has a phase with $x=0$ planes: it has a phase with $x=1$. In 2D, both insulating phases can be realized in models where there is a conserved quantity (e.g., $S_x$) that allows definition of ordinary Chern integers. A new feature in 3D is that the phases with $x_0=x_1=y_0=y_1=z_0=z_1=-1$ cannot be realized in this way. Since the results here are for Hilbert spaces of arbitrary dimension, they can be applied to many-body problems with an odd number of fermions if there are two periodic parameters in the Hamiltonian that are connected by time-reversal in the same way as the momentum components ($k_y, k_z$). Our derivation of $Z_2$ invariants helps explain spin Hall edge states: in 2D, just as Chern number predicts the number of edge states in the IQHE, the class of even (odd) Chern numbers in the bulk corresponds to edges with an even (odd) number of Kramers pairs of modes. Note that transport by these edge states will receive power-law, rather than exponential, corrections in voltage or temperature.

The existence of a 2D $Z_2$ invariant was also obtained by Haldane [12]. The bulk-edge connection has been derived when ordinary Chern integers are defined [13, 14, 15] (see also Ref. [16]). Recently preprints appeared on the 2D $Z_2$ invariant as an obstruction [14] or as a noninvariant Chern integral plus a formal integral on the EBZ boundary that is defined up to addition of an even integer [16]. Defining this integral is equivalent to our prescription of choosing any contraction to define a Chern integer. To our knowledge, the full counting of $Z_2$ invariants in 2D or 3D has not been obtained before.

Although whether graphene has sufficiently strong spin-orbit coupling to realize the topological insulator has been debated [14, 15], it is hoped that the understanding of $Z_2$ invariants developed here will stimulate searches in a wider class of materials, especially in 3D. The understanding of bulk $Z_2$ invariants in this paper, combined with the stability of total $Z_2$ to interactions and scattering at the edge [10, 20], shows that the topological insulator is a robust phase of matter with a deep connection to the quantum Hall effect.

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