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Topological invariants of time-reversal-invariant band structures

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The topological invariants of a time-reversal-invariant band structure in two dimensions are multiple copies of the $\mathbb{Z}_2$ invariant found by Kane and Mele. Such invariants protect the "topological insulator" phase and give rise to a spin Hall effect carried by edge states. Each pair of bands related by time reversal is described by one $\mathbb{Z}_2$ invariant, up to one less than half the dimension of the Bloch Hamiltonians. In three dimensions, there are four such invariants per band pair. The $\mathbb{Z}_2$ invariants of a crystal determine the transitions between ordinary and topological insulators as its bands are occupied by electrons. We derive these invariants using maps from the Brillouin zone to the space of Bloch Hamiltonians and clarify the connections between $\mathbb{Z}_2$ invariants, the integer invariants that underlie the integer quantum Hall effect, and previous invariants of $\mathcal{T}$-invariant Fermi systems.

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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 discussed graphene as a candidate system for this effect. Here $\mathbb{Z}_2 \equiv \mathbb{Z}/2\mathbb{Z}$ is the cyclic group of two elements ("even" and "odd"); it was argued that every band insulator in two dimensions belongs to either the even class or the odd class, where the even class describes ordinary insulators and the odd class describes topological insulators.

Both spin-orbit coupling and breaking of inversion symmetry are required to generate a topological insulator. A direct and experimentally relevant characterization of the invariant was given in terms of edge states at the boundary of a two-dimensional (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.

The goals of this paper are to explain how $\mathbb{Z}_2$ invariants arise in terms of the Thouless–Kohmoto–Nightingale–den Nijs (TKNN) integers[5,6] or "Chern numbers" familiar from the ordinary quantum Hall effect, and then to generalize the results to an arbitrary multiband band structure in two or three spatial dimensions. In the derivation below, we stress analogies to previous work[6] on understanding the integer quantum Hall effect (IQHE) via topological invariants of band structures in a commensurate magnetic field. Time-reversal-invariant ($\mathcal{T}$-invariant) 2D insulators are shown to have multiple $\mathbb{Z}_2$ invariants that are analogous to the band TKNN integers or Chern numbers in IQHE and can be understood using similar methods. This derivation differs from the two original descriptions 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. Intuitively, our results suggest that the topological insulator can be thought of as an IQHE that exists without a magnetic field or other $\mathcal{T}$ breaking.

Bands in a time-reversal-invariant fermion band structure come in pairs related by time reversal, with twofold Kramers degeneracies at certain special points of the Brillouin zone. We find that there are multiple $\mathbb{Z}_2$ invariants in such systems, associated with band pairs rather than individual bands, and perhaps most interestingly, four invariants per band pair in three dimensions. In two dimensions, the physical significance of these invariants is straightforward: just as two IQHE states with the same *sum* of Chern numbers for occupied bands are adiabatically connected, two $\mathcal{T}$-invariant band insulators are adiabatically connected if and only if they have the same $\mathbb{Z}_2$ sum of individual $\mathbb{Z}_2$ invariants for occupied band pairs.

The approach in this paper can be summarized 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. The importance of time-reversal symmetry is as follows: $\mathcal{T}$ symmetry means that only "half of the Brillouin zone" (which we define formally below as an "effective Brillouin zone," or EBZ) needs to be assigned Bloch Hamiltonians, as then the other half of the Brillouin zone is determined by symmetry. Then we study the topological classes of maps from the EBZ to the space of Bloch Hamiltonians.

The EBZ in two dimensions is almost but not quite a sphere: a key object in our analysis is a "contraction," defined below, that extends a mapping from the EBZ to one from the sphere. Once we have such a mapping from the sphere, then the ordinary Chern number is defined. Surprisingly, a given mapping from the EBZ has infinitely many inequivalent contractions in this sense; there are only two connected classes of band structures, for the case of two occupied bands connected by $\mathcal{T}$. These classes correspond to the ordinary insulator and the topological insulator. For one band pair, 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 details of band structure or the existence of additional commuting operators such as spin, and generalizes to multiple bands and higher dimensions.

We begin the derivation by recalling some facts about topological invariants of 2D band structures on the "magnetic Brillouin zone" (an effective unit cell in a lattice system with a magnetic field).[5,6] For 2D $\mathcal{T}$-breaking systems, in a nondegenerate band structure each band is associated with a TKNN integer that is invariant under smooth perturbations of the Bloch Hamiltonians. More precisely, if the Hilbert space of the nondegenerate Bloch Hamiltonians has dimension n, there are $n-1$ independent integer-valued invariants[6] because the invariants sum to zero. The Chern integer for a band is a Brillouin-zone integral involving the projection operator,[6]

$$n_i = \frac{i}{2\pi}\int_{BZ} \mathrm{Tr}(dP_i P_i dP_i), \quad P_i = |\psi_i\rangle\langle\psi_i|. \tag{1}$$

Here $dP_i = dx\partial_x P_i + dy\partial_y P_i$ and $dxdy = -dydx$. A powerful way to prove that these integer invariants are exhaustive[6] is by considering mappings of the torus to Bloch Hamiltonians, assumed nondegenerate. Denoting the space of such nondegenerate Hermitian matrices as $\mathcal{M}$, the TKNN integers follow from the homotopy groups

$$\pi_1(M) = 0, \quad \pi_2(M) = \mathbb{Z}^{n-1}, \tag{2}$$

where the second formula indicates $n-1$ copies of the infinite cyclic group $\mathbb{Z}$. The second result follows from the same exact sequence as used in the theory of topological defects.[7] For a pair of bands i,j that are degenerate with each other but with no other bands, there is a single integer-valued invariant[6] (total Chern number) obtained by replacing P_i in Eq. (1) with $P_{ij} = P_i + P_j$. In a time-reversal-invariant system, bands come in pairs, and the bands within a pair are required to be degenerate at some points by Kramers degeneracy. We define $\mathcal{C}$ as the set of Hermitian matrices allowing possible pair degeneracies (i.e., eigenvalues 1 and 2 may be degenerate, eigenvalues 3 and 4 may be degenerate, and so forth).

Now consider consequences of invariance under the time-reversal operator $\mathcal{T}$. For fermions, $\mathcal{T}^2 = -1$ and $\mathcal{T}$ is represented by an antiunitary operator Θ 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:

$$H(-k) = \Theta H(k)\Theta^{-1}. \tag{3}$$

Time-reversal invariance forces degeneracies at the four points where k goes to $-k$, and as a result the Bloch Hamiltonians in the band structure cannot be assumed nondegenerate (as in the IQHE case); instead, bands come in pairs related by time-reversal, and the only generic degeneracies are those within a pair.[23]

Figure 1 shows the original toroidal Brillouin zone and one possible EBZ (the right half of the original zone). Specifying the Hamiltonians for the points in the EBZ determines them everywhere. Note that *any* 2D Brillouin zone is topologically a torus: this follows from the requirement that multiple copies of the Brillouin zone tile the 2D reciprocal-lattice plane. There are four points of the 2D Brillouin zone that are invariant under $k \to -k$, and we assume below that the EBZ boundaries are chosen to connect pairs of these points. The Bloch Hamiltonians can be specified independently on the EBZ except at the boundaries, where points are conjugate under $\mathcal{T}$ as shown. Clearly points at which $k=-k$, such as Γ, **A**, **B**, **C** in Fig. 1, are special: at these points the Bloch Hamiltonian commutes with Θ. We denote the set of such Hamiltonians that commute with Θ, with the additional assumption of no degeneracies other than the twofold degeneracies required by $\mathcal{T}$, as $\mathcal{Q}$ (Ref. 8). The twofold Kramers degeneracies exist because, for any energy eigenstate $|\psi\rangle$, $T|\psi\rangle$ is an orthogonal state with the same energy (since $T^2 = -1$). $\mathcal{T}$ invariance requires an even number of bands $2n$, so $\mathcal{Q}$ consists of $2n \times 2n$ Hermitian matrices for which H commutes with Θ. $\mathcal{Q}$ is the even subspace in the language of Ref. 1.

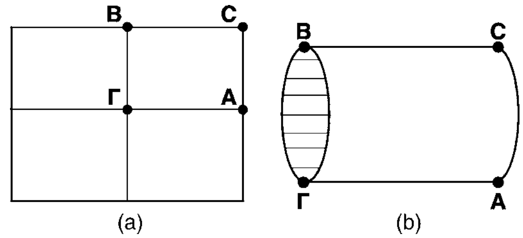

FIG. 1. The topology of the effective Brillouin zone (EBZ): if the original Brillouin zone is the torus in (a), then $\mathcal{T}$ invariance reduces the independent degrees of freedom to live on half the Brillouin zone; one choice of "half the Brillouin zone" is the manifold in (b) (here we have chosen the right half of the original Brillouin zone to form an EBZ). Points on the boundary circles that are connected by horizontal lines are conjugate under $\mathcal{T}$; the points Γ, A, B, C are self-conjugate, and their Bloch Hamiltonians are therefore in the even subspace $\mathcal{Q}$. Note that the EBZ has been chosen so that each boundary passes through two of these special points.

In general, a $\mathcal{T}$-invariant system need not have Bloch Hamiltonians in $\mathcal{Q}$ except at these special points as long as inversion symmetry is broken, which allows $H(k) \neq H(-k)$. 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 for a single nondegenerate band: writing $P_i = |\psi_i\rangle\langle\psi_i|$,

$$\begin{aligned} n_i &= \frac{i}{2\pi}\,\mathrm{Im}\int [\langle\partial_x\psi_i|\partial_y\psi_i\rangle + \langle\partial_x\Theta\psi_i|\partial_y\Theta\psi_i\rangle] \\ &= \frac{i}{2\pi}\,\mathrm{Im}\int [\langle\partial_x\psi_i|\partial_y\psi_i\rangle + \langle\partial_y\psi_i|\partial_x\psi_i\rangle] = 0. \end{aligned} \tag{4}$$

The total Chern number similarly vanishes for two degenerate bands connected by $\mathcal{T}$ in a $\mathcal{T}$-invariant system, but there is still a topological invariant,[1] as we explain.

As a quick example of homotopy arguments, suppose that inversion symmetry is unbroken, which implies that the Bloch Hamiltonians are everywhere in $\mathcal{Q}$. Any mapping of

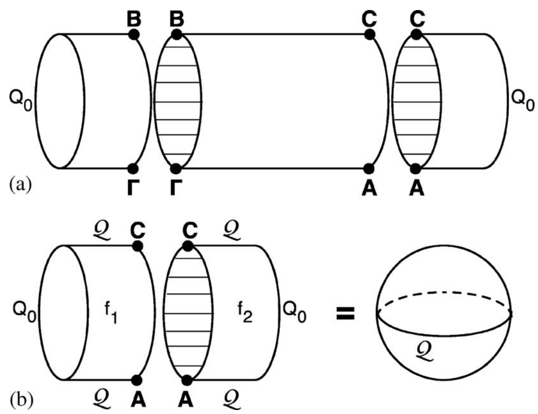

FIG. 2. (a) Contracting the extended Brillouin zone to a sphere. (b) Two contractions can be combined according to Eq. (5) to give a mapping from the sphere, but this sphere has a special property: points in the northern hemisphere are conjugate under $\mathcal{T}$ to those in the southern hemisphere, in such a way that overall every band pair's Chern number must be even.

the torus T^2 to $\mathcal{Q}$ 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 $\mathcal{T}$-conjugate points together in Fig. 1(b)]: the classes of such mappings are given by[8] $\pi_2(\mathcal{Q})=0$. Hence there is no homotopy invariant for 2D band structures with both $\mathcal{T}$ and inversion symmetry, although $\pi_4(\mathcal{Q})\neq 0$ and higher-dimensional invariants can exist.

Now consider possible invariants without inversion symmetry. We seek to classify mappings from T^2 to Bloch Hamiltonians that are consistent with $\mathcal{T}$ invariance and have no accidental degeneracies. Such a mapping is determined by a mapping from the EBZ, i.e., a mapping from the cylinder C to $\mathcal{C}$ with certain conditions on the two circular boundaries reflecting time reversal. The image of a boundary point must be the Θ conjugate of the image of the point related by $k\leftrightarrow -k$.

We show that any mapping from C to $\mathcal{C}$, even if the elements at a boundary are not all the same, can be deformed ("contracted") to one in which the boundary elements are identical to an arbitrary reference element $Q_0\in\mathcal{Q}$ [Fig. 2(a)]; the resulting map from the *sphere* has well-defined Chern numbers. It is required that at each stage of the contraction, the boundary has the same conjugacy under $\mathcal{T}$ as the original EBZ boundary, to guarantee that two maps from the EBZ that can be contracted to maps from the sphere with the same Chern numbers are homotopic (deformable to each other).

Then it is shown that different contractions differ by arbitrary even Chern numbers, so that there are only two invariant classes per band pair according to whether the Chern number with any contraction is an odd or even integer. A contraction is formally defined as a mapping from the cylinder with angular coordinate $\theta\in[0,2\pi)$ and length coordinate $\lambda\in[0,1]$ to $\mathcal{C}$, $f(\theta,\lambda)$, such that $f(\theta,\lambda)$ and $f(2\pi-\theta,\lambda)$ are $\mathcal{T}$ 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 on the EBZ boundary, while $f(\theta,1)=Q_0$ is constant. If both boundaries are contracted, the resulting sphere has a well-defined Chern number n_B^i for each pair i of bands. The existence of one contraction follows from $\pi_1(\mathcal{C})=0$: contract one side of the boundary circle to the point Q_0, then determine the other side by $\mathcal{T}$ conjugacy.

Many topologically inequivalent contractions exist, and this reduces the integer-valued Chern numbers 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 $g(\theta,\lambda)$, again with coordinates $\theta\in[0,2\pi)$, $\lambda\in[0,1]$, which combines contractions f_1 and f_2 [Fig. 2(b)]:

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

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 $\mathcal{T}$ symmetry from the contracted half of the Brillouin zone, which in its interior has no $\mathcal{T}$ symmetry relating different values of θ: the values of g at the points (θ,λ) and $(2\pi-\theta,\lambda)$ are $\mathcal{T}$ conjugate.

Now we show that g has *even* Chern numbers. This can be verified in two steps: map the equator of the sphere S to the reference element Q_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 for each band pair 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 $\mathcal{T}$ of θ 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 Eq. (4). Another minus sign comes from $\mathcal{T}$ conjugacy, as in Eq. (4), so overall the contributions from the two hemispheres add. Finally, the change Δn_B^i in the band pair Chern numbers n_B^i that results by changing from contraction f_1 to contraction f_2 is given by the Chern numbers n_g^i of the mapping g (note that f_1 appears in g with one of its coordinates reversed, but not the other, so that the sign of its Chern number is flipped). Since the n_g^i are twice those of one hemisphere n_S^i,

$$\Delta n_B^i = n_g^i = 2n_S^i. \tag{6}$$

Finally, in a band structure with n pairs of bands, there is one integer for each pair with a zero sum rule. Hence there is one $\mathbb{Z}_2$ invariant for each band pair, with a $\mathbb{Z}_2$ zero sum rule; there must be an even number of "odd" pairs in a complete band structure.

We now sketch the generalization to three-dimensional Brillouin zones, where there are significant differences between $\mathbb{Z}_2$ invariants and the 3D integer-valued TKNN invariants.[5,6] There are four independent $\mathbb{Z}_2$ invariants per pair of bands, even though there are only three Chern numbers for a pair of degenerate bands. The set of mappings from the Brillouin zone T^3 to $\mathcal{C}$ is determined by three ordinary Chern numbers since $\pi_3(\mathcal{C})=0$: the three integers correspond to the xy, yz, and xz planes.[6]

Now consider possible $\mathbb{Z}_2$ invariants for a time-reversal-invariant system in three dimensions. Suppose that the Brillouin zone is $x,y,z \in [-1,1]$, and construct an EBZ by taking the part of this three-torus with $z \geq 0$. Then slices at constant z for $0<z<1$ have the topology of the torus T^2, while at $z=0$ and $z=1$ there are additional $\mathcal{T}$ constraints that reduce the degrees of freedom to the 2D BZ. The $\mathcal{T}$ constraint means that the xy Chern number is zero.

The EBZ boundaries at $z=0$ and $z=1$ are characterized by one $\mathbb{Z}_2$ invariant each: one boundary may be even while the other is odd because the boundary slices have the same Chern number (zero) and thus are homotopic as maps to $\mathcal{C}$ in the EBZ interior. Once the two $\mathbb{Z}_2$ invariants at the boundaries are fixed, two contractions of an original 3D EBZ to the torus T^3 differ by two even Chern numbers, one for the xz slices and one for the yz slices. These are even because a slice of the contraction has the same symmetries that force even Chern numbers in the 2D case. There are four additive $\mathbb{Z}_2$ invariants per band pair in three dimensions and 16 insulating phases.

To understand these four invariants using the original Brillouin zone, note that the six planes $x=0$, $x=\pm 1$, $y=0$, $y=\pm 1$, $z=0$, $z=\pm 1$ have the symmetries of the 2D BZ and hence have a $\mathbb{Z}_2$ invariant. If the six invariants with values ± 1 are x_0, x_1, y_0, y_1, z_0, z_1, then there are two relations $x_0 x_1 = y_0 y_1 = z_0 z_1$. As a 3D example, a model can be designed on the 3D NaCl lattice to reduce to a previously introduced[9] 2D square lattice topological insulator in the $k_y=0$ or $k_z=0$ planes: it has a phase with $y_0=y_1=z_0=z_1=-1$, $x_0=x_1=1$. In two dimensions, both insulating phases can occur in models with a conserved quantity (e.g., S_z) that allows a definition of ordinary Chern integers. In three dimensions, the eight 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 apply to many-body problems with an odd number of fermions[8] if there are two periodic parameters in the Hamiltonian that are connected by time reversal in the same way as the momentum components (k_x, k_y). In two dimensions, just as the Chern number predicts the number of edge states in the IQHE,[10] the class of even (odd) Chern numbers in the bulk corresponds to edges with an even (odd) number of Kramers pairs of modes.

A 2D $\mathbb{Z}_2$ invariant was also obtained by Haldane.[11] The bulk-edge connection has been derived when ordinary Chern integers are defined[12–14] (see also Ref. 15). Recent papers define the 2D $\mathbb{Z}_2$ 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.[15] Defining this integral is equivalent to our prescription of choosing any contraction to define a Chern integer. The full counting of $\mathbb{Z}_2$ invariants in two or three dimensions has not been obtained previously.

These bulk invariants and the stability of total $\mathbb{Z}_2$ to edge interactions and scattering[16–18] confirm that the topological insulator is a robust phase with a deep connection to the quantum Hall effect.

Recently, consistent results in three dimensions were found by others.[19,20] Other important results include 3D examples with nonzero fourth invariant $z_0 z_1$ (Ref. 21) and an algorithm to obtain the invariants.[22]

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[23] Note that just as touching bands can transfer the Chern number in the IQHE, interpair degeneracies allow $\mathbb{Z}_2$ to be transferred between pairs with total $\mathbb{Z}_2$ conserved.