Topological phases and the quantum spin Hall effect in three dimensions

Rahul Roy
Department of Physics and Astronomy, McMaster University, Hamilton, Ontario, Canada L8S 4M1
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We show the existence of topological phases of Bloch insulators with time-reversal symmetry in three dimensions. These phases are characterized by topological Z_2 invariants whose stability is studied using band-touching arguments. Unlike insulators which break time-reveral symmetry, some of these topological phases are intrinsically three dimensional. The number of invariants (four) needed to specify the phase of these insulators also differs from the time-reversal-breaking case. The relation between these phases and the quantum spin Hall effect in three dimensions is investigated.

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Topological phases, the most well known of which are perhaps the integer and fractional quantum Hall states, are an exciting set of condensed-matter systems. The integer quantum Hall (IQH) phases can be characterized by a topological invariant; have robust edge states and quantized response properties; and can be realized in simple noninteracting models which *break* time-reversal symmetry (TRS).[1,2]

Recently, it was realized that topological phases can also exist in simple two-dimensional (2D) band insulators which preserve TRS.[3–5] These insulators have two phases and are said to be characterized by a topological Z_2 invariant. The topological phases with a nontrivial value of this invariant have robust edge states similar to the IQH states. The edge states in these phases, unlike in the IQH effect, carry no net charge current. They can, however, carry a spin current. Indeed, it is in connection with the spin Hall effect that these topological phases were unearthed.

Topological phases also exist in three dimensions in insulators which break TRS.[6–8] It is interesting, therefore, to investigate whether such phases can also exist in systems which *do not* break TRS in three dimensions. We address this question in this paper. Indeed, we shall see that there are topological phases of time-reversal-symmetric insulators in three dimensions that have no two-dimensional analogs. In contrast, the IQH phases in three dimensions are directly related to the IQH phases in two dimensions.[6–8] We propose the three-dimensional (3D) quantum spin Hall effect (QSHE) and investigate the connection between the topological phases in three dimensions and the QSHE.

We first discuss the Z_2 invariant in two dimensions using arguments based on band-touching and adiabatic continuity. These help to provide an easy-to-follow and intuitive alternative understanding of the invariant. Using the framework provided by these arguments, we then study the topological phases of three-dimensional insulators and provide a classification of these phases.

I. Z_2 INVARIANT IN TWO DIMENSIONS

The Z_2 invariant associated with the topological phases was first studied in terms of the zeroes of the Pfaffian of the time-reversal operator among bands.[4] A different approach to the Z_2 invariant was taken in Ref. 9 which clarified the connection between the invariant and the edge states of the system and put the Z_2 classification on a firmer mathematical footing. In that work, the Z_2 invariant was expressed in terms of the Thouless-Kohmoto-Nightingale-de Nijs (TKNN) numbers[1,10] of wave functions which form a basis for the vector space spanned by the occupied bands. The TKNN numbers are integrals of the Berry curvature of the wave functions in momentum space. If $\{c_n\}$ is the set of TKNN numbers of these wave functions, then the Z_2 invariant is given by the sum of the positive numbers in this set modulo two.

The topological Z_2 invariant must be invariant under adiabatic transformations of the Hamiltonian as well as continuous transformations of the basis wave functions which keep the ground state unchanged. To study the effects of both types of transformations, it is convenient to associate with the system a Hamiltonian of a particularly simple form, which has the property that its ground state is the same as that of the original system or is one which may be obtained by an adiabatic deformation of the original Hamiltonian of the system.

Let us first consider the case when there are two occupied bands in the ground state. We associate with the ground state a Hamiltonian[11] of the form

$$H = H_1 + H_2, \tag{1}$$

where

$$H_1 = \int_{\mathrm{BZ}} d^2k[E_1(\mathbf{k})|u_1\rangle\langle u_1| + E_2(\mathbf{k})|u_2\rangle\langle u_2|], \tag{2}$$

$$H_2 = \int_{\mathrm{BZ}} d^2k \sum_{n>2} E_n(\mathbf{k})|u_n\rangle\langle u_n|. \tag{3}$$

Here, n is the band index and the integral is taken over the Brillouin zone. The energies E_1 and E_2 are less than zero while $E_n>0$ for $n>2$ and the Fermi energy E_f is equal to zero. Further, we assume that the Hamiltonian H is such that $|u_1(\boldsymbol{k})\rangle$ and $|u_2(\boldsymbol{k})\rangle$ are locally continuous functions of the momentum variables and can be uniquely defined.[12]

The time-reversal symmetry of the Hamiltonian leads to the condition $E_1(\mathbf{k})=E_2(-\mathbf{k})$ and

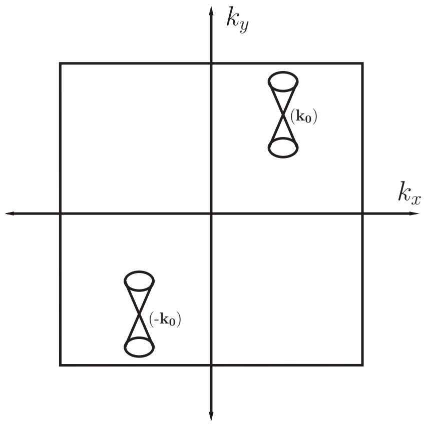

FIG. 1. A schematic figure showing the diabolical points in the spectrum of the associated Hamiltonian.

$$\Theta|u_1(\boldsymbol{k})\rangle = |u_2(-\boldsymbol{k})\rangle, \quad \Theta|u_2(\boldsymbol{k})\rangle = -|u_1(-\boldsymbol{k})\rangle, \tag{4}$$

where Θ is the time-reversal operator.

To study the effect of either an adiabatic variation of the system or a continuous change in the basis, we consider an adiabatic variation in the associated Hamiltonian. Let $H(t)$ be a continuous set of Hamiltonians such that $H(t)$ can be written as a sum of $H_1(t)$ and $H_2(t)$ which have the same properties as H_1 and H_2 in Eq. (1) specified above. The TKNN invariants or the Chern numbers for the two bands are then individually conserved, and the sum of these two Chern numbers is zero. (This follows from homotopy arguments of the form presented in Ref. 9 or by a direct computation of the Chern number in terms of the Berry phase by using the TKNN formulae.[1] A simple physical argument for this follows from the observation that the Hall conductivity of a system with time-reversal invariance is zero. Then using the standard TKNN result,[1] which relates the Hall conductivity to the sum of the Chern numbers, it follows that the sum of the Chern numbers of these bands is zero.) It follows that the quantity defined as $|c| \bmod 2$ where c is the TKNN number of either band is unchanged through such an adiabatic transformation.

Since the invariant is unaffected by any process where the individual wave functions are continuously transformed, we now consider a transformation of the associated Hamiltonian where the Chern numbers of the bands can change. Suppose that an isolated diabolical point occurs in the three-dimensional parameter space at a point $(t_0, \mathbf{k}_0)$. The bands are then no longer continuous at this point. Due to time-reversal invariance, a diabolical point must also occur at $(t_0, -\mathbf{k}_0)$ as shown in Fig. 1. A two-level degeneracy is generic while a higher-level degeneracy is not.[13] Without the loss of generality, one can thus write $\tilde{H}_1(t)$ in the vicinity of the degeneracy points as

$$\tilde{H}_1(t,\mathbf{k}) = \mathbf{m}(t,\mathbf{k}) \,.\, \sigma + \frac{E_1+E_2}{2} I, \tag{5}$$

where the two indices of the σ matrices correspond to the two bands $|u_1\rangle$ and $|u_2\rangle$. Time-reversal invariance then dictates that

$$\mathbf{m}(t,-\mathbf{k}) = -\mathbf{m}(t,\mathbf{k}). \tag{6}$$

At the degeneracy point $\mathbf{m}(t_0,\mathbf{k}_0)=\{0,0,0\}$.

As the parameter t is further changed, the bands may split apart again. However, as they separate, the bands might now have a new set of Chern numbers whose sum has to be the same as before the band collision (zero).[14] The degeneracy points may be visualized as monopoles which flow in and out of the bands.

If one sets $\vec{\omega}=\mathbf{m}/|m|$, then the Chern number exchange between the bands is given by[15]

$$n(x_0) = \pm \frac{1}{4\pi}\int_{\Sigma_j} \langle \vec{\omega}| d\vec{\omega} \wedge d\vec{\omega}\rangle, \tag{7}$$

where Σ_j is the surface of a small sphere enclosing the degeneracy point in the three-dimensional space of points (t,k_x,k_y). From the property of time-reversal invariance, it follows that the Chern number exchange between a band and its time-reversed counterpart at the two points $(t_0,\mathbf{k}_0)$ and $(t_0,-\mathbf{k}_0)$ is exactly the same (in magnitude and sign). Hence the total Chern number exchanged between bands is always an even number.

For a system with multiple occupied pairs of bands in the ground state, two kinds of "band collisions" can occur: (a) a degeneracy between a band and its time-reversed counterpart and (b) a degeneracy between two bands which are not related by time reversal. In the second type of band collision, the fact that the time-reversed pairs before and after collision have opposite Chern numbers, which add up to zero for each pair, implies that if a band $|\alpha\rangle$ changes its Chern number by n_α then the Chern number of $\Theta|\alpha\rangle$ changes by $-n_\alpha$. These preserve the net Z_2 invariant[9]

$$E = \left|\sum_{c_n>0} c_n\right| \bmod 2, \tag{8}$$

where the summation is over the set of bands which have positive Chern numbers. The first kind of process also preserves this invariant as evident from the arguments presented earlier for the model with two occupied bands. These band-touching arguments provide an alternative and intuitive understanding of the Z_2 invariant in two dimensions. In three dimensions, we will map the topological phases of insulators by showing that certain quantities which are invariant under adiabatic transformations may be associated with the ground states of the different phases.

II. TOPOLOGICAL PHASES IN THREE DIMENSIONS

The Brillouin zone in three dimensions is topologically equivalent to the torus T^3 and may be parameterized by the set of points $\{(x,y,z)|-1 \geq x,y,z \leq 1\}$ such that the time-reversal operator Θ maps the Bloch wave functions at the point (x,y,z) to those at the point $(-x,-y,-z)$. We consider separately two different cases:

(1) let us choose an associated Hamiltonian with the same ground-state wave function as the system in consideration that can be written as a sum H_1+H_2 as in Eq. (1) and such that the corresponding eigenkets of H_1 are locally continuous

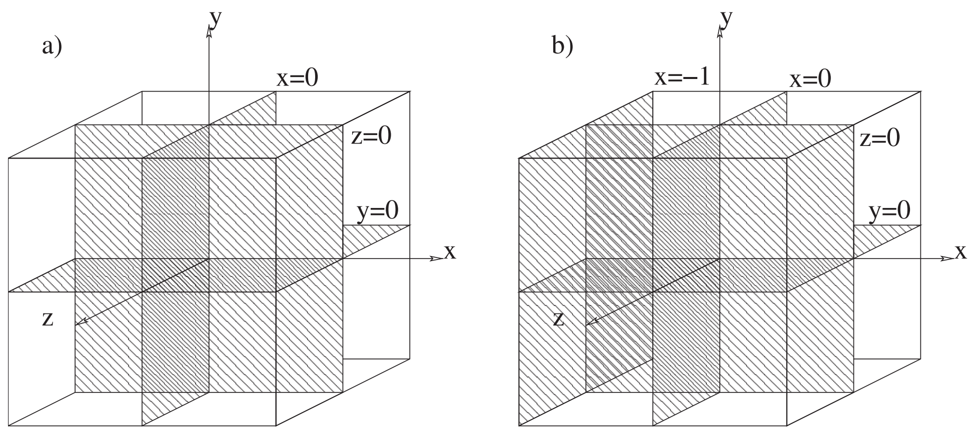

FIG. 2. A representation of the Brillouin zone for a three-dimensional insulator. The two-dimensional planes whose Z_2 invariants specify the topological phase are shaded for (a) the case when there are no diabolical points, and (b) when there are diabolical points in the spectrum of the associated Hamiltonian.

at all points in the Brillouin zone. The Bloch wave functions on the planes $\{x,y,z=0;\ x,y,z=1\}$ get mapped on to themselves and satisfy the symmetries of the Bloch wave functions in two dimensions. We can thus define a set of three Z_2 invariants E_{yz},E_{zx},E_{xy}, one for each of the planes $x=0$, $y=0$, and $z=0$ [Fig. 2(a)],

$$E_{xy} = \left| \sum_{c_n^{xy}>0} c_n^{xy} \right| \bmod 2, \tag{9}$$

$$E_{yz} = \left| \sum_{c_n^{yz}>0} c_n^{yz} \right| \bmod 2, \tag{10}$$

$$E_{zx} = \left| \sum_{c_n^{zx}>0} c_n^{zx} \right| \bmod 2, \tag{11}$$

where $c_n^{xy},c_n^{yz},c_n^{zx}$ are the Chern numbers of the nth occupied band for the different planes. Further, since by assumption there are no diabolical points in the Brillouin zone, the Chern numbers and hence the Z_2 invariant associated with the plane $x=1$ is identical to the Z_2 invariant for the plane $x=0$. Similar statements hold for the other two planes.

Let us now consider an adiabatic continuation of H_1 where band touchings occur and split into Dirac points. These can be thought of as monopoles of opposite charge which can recombine after relative displacement through a reciprocal lattice vector as explained in Ref. 16. Due to the constraints of time-reversal invariance, however, the Chern numbers can only change in such a way that the Z_2 invariants for the 2D planes are preserved in the process. There are thus three independent Z_2 invariants and a specification of these serves to identify the topological phase in this case.

(2) Now consider ground states where the associated Hamiltonian has isolated diabolical points at which the eigenstates cannot be continuously defined. Let us call sets of points of the form

$$T^3_{(1/2)z+} = \{(x,y,z) | 0 \geq z \leq 1, -1 \geq x,y \leq 1\},$$

$$T^3_{(1/2)z-} = \{(x,y,z) | -1 \geq z \leq 0, -1 \geq x,y \leq 1\},$$

and similarly defined sets for the x and the y directions, 3D half tori. We further divide these half tori into quarter tori which are defined by the intersection of half tori such as $T^3_{(1/4)z-,x-} = T^3_{(1/2)z-} \cap T^3_{(1/2)x-}$. The half and quarter tori come in pairs such as $\{T^3_{(1/2)z+},\ T^3_{(1/2)z-}\}$ which get mapped onto each other under the projection of the time-reversal operator. We call these complementary pairs. We consider a single pair of time-reversed bands and a set of diabolical points (which may be regarded as monopoles) which do not lie at the surfaces of any of the quarter tori. Time reversal maps these monopoles in quarter tori to monopoles in their complementary quarter tori such that if a band collides with its time-reversed counterpart, the charge that flows in at one monopole to a band is the opposite of the charge that flows in at the other monopole. If there is an odd number of such monopoles in the half torus $T^3_{(1/2)z-}$, then the Z_2 indices of the plane $z=0$ and the plane $z=1$ are different while they are the same if there is an even number of monopoles.[17] Since these Z_2 indices are homotopically stable, at least one pair of monopoles in the Brillouin zone cannot recombine and vanish in the first case while all the monopoles can recombine and vanish in the second. In the first case, therefore, the monopoles are thus trapped and hence stable. Further, from the mapping of monopoles to their counterparts in quarter tori, one can see that if a certain half torus has an odd number of monopoles, so must all the other half tori. Hence the Z_2 invariants of the planes $y=1$ and $x=1$ are uniquely determined from the Z_2 invariants of the planes $x=0$, $y=0$, $z=0$, and $z=1$. Four Z_2 invariants are thus needed to specify the topological phase.

In the case of multiple bands, one may simply evaluate the monopole charge flowing into half the set of filled bands, say, for instance, the set of bands with positive Chern numbers and half the set of those with Chern number zero. The set of bands chosen has to be such that no two elements of the set map onto each other under time reversal.

A complete set of Z_2 invariants is thus obtained, for example, by choosing the Z_2 invariants of the planes $x=0$, y

$=0$, $z=0$, and the plane $x=1$ as shown in Fig. 2(b). Alternatively, one may take the fourth Z_2 invariant to be the difference of the Z_2 invariants of the planes $x=1$ and $x=0$. The fourth Z_2 invariant defined in this way is nontrivial when there is an odd number of monopoles while it is zero when there is an even number of monopoles. The phases that have no diabolical points in the associated Hamiltonian thus correspond to a trivial value of the fourth Z_2 invariant. The phases associated with a nontrivial value of the fourth Z_2 invariant cannot be constructed by stacking layers of a 2D QSHE system as opposed to the integer quantum Hall effect (IQHE) case. Indeed, four topological invariants are needed to characterize insulators with TRS while three suffice in the case when TRS is broken.[18] This is one of the key differences between the two cases. When time-reversal symmetry is broken, such as in the presence of an external magnetic field, the Z_2 indices are no longer invariant and hence, the trapped monopoles may vanish.

Topological invariants of insulators with time-reversal symmetry in three dimensions have been discussed in Refs. 19–21. Four topological invariants and 16 phases for time-reversal-invariant insulators in three dimensions were deduced in these works which are in agreement with the current work. Examples of the nontrivial topological phases have also appeared.[21]

III. QUANTUM SPIN HALL EFFECT IN THREE DIMENSIONS

So far, we have not connected the topological phases in three dimensions proposed above to measurable transport properties. In two dimensions, the topological phases are associated with the QSHE, i.e., with models in which the spin Hall response is quantized in units of e^2/h. We first show that the occurrence of a three-dimensional QSHE which is characterized by a quantized spin Hall conductance in three dimensions is possible. We then discuss the connections between the topological phases discussed above and the QSHE.

The possibility of the three-dimensional quantum Hall effect has been pointed out by Halperin *et al.*[6–8] The three independent Chern numbers for filled bands in three dimensions play the same role in determining the quantized Hall response as the single Chern number does in two dimensions. When time-reversal symmetry is preserved, models have been proposed where spin is a good quantum number (the Hamiltonian commutes with s_z) and where a quantized spin Hall current response is obtained in two dimensions.[3,5] The spin-current response arises from equal contributions from the up and down spins $\mathbf{J}_s=\frac{\hbar}{2e}(\mathbf{J}_\uparrow-\mathbf{J}_\downarrow)$, each of which has a quantized response to the external electric field, but in opposite directions. A stack of layers of such a 2D material with weak interlayer coupling such that the Fermi energy lies in a band gap, will thus lead to a quantum spin Hall effect in three dimensions as long as the spins are decoupled. The spin-conductivity tensor can be written in the form

$$\sigma_{ij}^{s}=\frac{e}{8\pi^2 h}\epsilon_{ijk}G_k, \qquad (12)$$

where $\vec{G}$ is a reciprocal lattice vector. A Hamiltonian which displays such a quantized response in the $k_z=0$ and $k_y=0$ planes can be obtained by a simple generalization of the two-dimensional model presented in Ref. 22. The stability of the edge states is governed by the three-dimensional Z_2 invariants presented earlier, even though the spin Hall conductivity itself is not expected to be quantized when terms, which mix up and down spins, are present. Since a nontrivial value of the fourth Z_2 index is not possible without band degeneracies that change the Z_2 invariants of a pair of bands across a half torus, a quantized spin Hall response can only be obtained when this index is zero.

We have thus classified the phases of band insulators with time-reversal symmetry in three dimensions and found topological phases which are classified by topological Z_2 invariants. We also introduced the phenomenon of the quantum spin Hall effect in three dimensions and discussed the connection between this phenomenon and the topological phases. Since the topological phases are related directly to the Chern numbers and these are, in turn, connected with the presence of robust edge states,[23] a natural connection between these topological phases and the existence of robust edge states is expected.

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