Characterization of three-dimensional topological insulators by two-dimensional invariants

Rahul Roy
Rudolf Peierls Centre for Theoretical Physics, 1 Keble Road,
Oxford OX1 3NP, UK
E-mail: r.roy1@physics.ox.ac.uk

New Journal of Physics 12 (2010) 065009 (6pp)
Received 5 October 2009
Published 17 June 2010
Online at http://www.njp.org/
doi:10.1088/1367-2630/12/6/065009

Abstract. The prediction of nontrivial topological phases in Bloch insulators in three dimensions has recently been experimentally verified. Here, I provide a picture for obtaining the $\mathbb{Z}_2$ invariants for a three-dimensional (3D) topological insulator by deforming suitable 2D planes in momentum space and by using a formula for the 2D $\mathbb{Z}_2$ invariant based on the Chern number. The physical interpretation of this formula is also clarified through the connection between this formulation of the $\mathbb{Z}_2$ invariant and the quantization of spin Hall conductance in two dimensions.

Contents

1. Two dimensions
2. Three-dimensional insulators
Acknowledgments
References

Insulators with weak inter-electronic interactions in crystalline materials are well described by band theory. The energy eigenstates can be grouped into Bloch bands and the presence of a gap at the Fermi energy prevents charge transport in the bulk since filled bands do not contribute to electronic transport. Since the discovery of the quantum Hall effect [1], however, it has been known that materials that have a bulk gap in their single-particle spectra may nevertheless have gapless edge modes, through which charge transport may take place. Various theoretical studies, an incomplete list of which includes [2]–[6], have helped to explain the quantization of the conductance, the connection between the bulk Hamiltonian and the Hall conductance, and the robustness and role of the edge states in the quantum Hall effect.
Recently, a set of novel topological phases that are somewhat similar to the quantum Hall phases have been proposed to exist in ordinary insulators with unbroken time reversal symmetry (TRS). (From here on, unless stated otherwise, we shall restrict ourselves to a discussion of band insulators with unbroken TRS.) In two dimensions, there are two distinct topological phases [7] characterized by a single $Z_2$ invariant, whereas in three dimensions, 16 topological phases characterized by four topological $Z_2$ invariants [8]–[10] have been proposed to exist in non-interacting systems. These topological phases have been detected in HgTe quantum wells surrounded by CdTe in two dimensions [11, 12] and in Bi$_{1-x}$Sb$_x$ alloys in three dimensions [13, 14] among the other compounds. Like in the quantum Hall effect, the topologically nontrivial phases of insulators with TRS have gapless edge modes that are robust to small perturbations. Topological phase transitions between these phases have been studied in [15].

While in two dimensions the analogy with the integer quantum Hall effect leads to a simple picture for the topological phases and the $Z_2$ invariant, in three dimensions, the picture is far more complicated. This is, in part, due to the fact that unlike the integer quantum Hall effect, in three-dimensional (3D) materials with unbroken TRS, while three of the $Z_2$ invariants are analogous to the 2D $Z_2$ invariants, there is a fourth $Z_2$ invariant which is intrinsically 3D. Insulators with a nontrivial value of this fourth invariant have a description in terms of an effective field theory containing a $\theta$ term, which successfully describes the physics of the boundary [16]. In this work, I provide a different argument for counting the number of different topological invariants and thus the number of different topological phases in 3D insulators. Since the picture relies on invariants for 2D topological insulators, I will briefly review this case as well. A physical interpretation of the invariant as formulated in terms of Chern numbers in two dimensions is also provided.

1. Two dimensions

The original approach to the topological invariant in two dimensions was based on counting the zeroes of a function calculated from the Pfaffian of a certain matrix [7]. A different approach developed by the author was based on the obstruction of the vector bundle of wave functions on the torus to being a trivial bundle [17]. This yielded a formula involving the Chern number of half the occupied bands. Subsequent work using the obstructions approach and physical ideas related to charge polarization led to a formula involving an integral of the Berry curvature of all the bands, but restricted to half the Brillouin zone (also called the effective Brillouin zone (EBZ)) [18]. In other related work, the topological phases in two dimensions were studied by deforming maps from the EBZ to the space of Bloch Hamiltonians with unbroken TRS, $\mathcal{C}$, to maps from a sphere or a torus to $\mathcal{C}$ ([8]). The formula involving the integral over the EBZ in [18] has been adapted to numerical evaluations [19], while the formula in terms of the Chern number has the advantage of having a direct link to the edge state physics and the integer quantum Hall effect. A brief review of the latter formulation is provided below.

The Hamiltonian of a Bloch insulator has single-particle eigenstates, which are either occupied or unoccupied depending on their energy relative to the Fermi energy. The spectral projection operator is defined as the operator that projects single-particle states onto the space of occupied states. It can thus be written as a sum, $P = \sum_i |u_i\rangle\langle u_i|$, where the $|u_i\rangle$ are the occupied eigenkets. Thus the projection operator (for a finite periodic system) can be written as $P = \sum_{k_x,k_y} P(k_x,k_y)$, where the sum is over reciprocal lattice vectors lying in the Brillouin zone.
As was argued in [17], in materials with TRS, the spectral projector, \( P \), can be written in the form
\[
P(k_x, k_y) = P_1(k_x, k_y) + P_2(k_x, k_y),
\]
where the operators \( P_1 \) and \( P_2 \) are well defined, continuous functions of the momentum variables and are related through TRS:
\[
P_1(k_x, k_y) = \Theta P_2(-k_x, -k_y) \Theta^{-1}.
\]
Here, \( \Theta \) is the time reversal operator that acts on the spin degrees of freedom and is anti-linear. The choice of \( P_1 \) and \( P_2 \) is not unique. We further assume that a choice of \( P_1 \) and \( P_2 \) can be made such that \( P_1 \) and \( P_2 \) are smooth at all points in the 2D Brillouin zone (see [17, 21]).

For every value of \( k \), \( P(k) \) projects onto a complex vector space. We thus obtain a vector bundle over momentum space. The first Chern number of this bundle, which we denote by \( \mu(P) \), can be written in the form [20]
\[
\mu(P) = \frac{1}{2\pi i} \int dk_x dk_y \text{Tr} \left( P \left( \frac{\partial P}{\partial k_x} \frac{\partial P}{\partial k_y} - \frac{\partial P}{\partial k_y} \frac{\partial P}{\partial k_x} \right) \right).
\]

The first Chern number vanishes for \( P \) in topological insulators due to TRS, i.e. \( \mu(P) = 0 \). However, it was shown that \( \nu(P) = |\mu(P_1)| \mod 2 \) is a topological invariant [17] and is independent of the choice of \( P_1 \).

Consider the subset of gapped Bloch Hamiltonians that conserve the \( z \)-component of the spin, i.e. Hamiltonians in which there are no terms that turn up spins into down spins. The energy eigenstates can be decomposed into spin-up and spin-down bands. Hamiltonians in this class with a bulk gap will always have a quantized spin Hall conductance (which could be zero).

The \( Z_2 \) topological classification tells us that Hamiltonians of the even- and the odd-quantized spin Hall effects are distinct even when we allow spin-mixing terms in the Hamiltonian. In terms of the spin Chern number \( C_s \), which can be defined for such models [22], the \( Z_2 \) invariant is \( |C_s/2| \mod 2 \).

In other words, if we allow the terms that cause spin mixing, the Hamiltonians with an even spin Hall effect can all be transformed into one another through adiabatic changes in parameter space and those with an odd spin Hall effect can similarly be adiabatically transformed into one another. However, no member of the odd spin Hall conductance class can be transformed into any member of the even spin Hall conductance in a continuous way such that TRS is protected and the system is gapped at all points of the transformation. Further, any general Bloch Hamiltonian (with the same Hilbert space and which has the same number of occupied bands) that preserves TRS may be adiabatically transformed to Hamiltonians of precisely one of the two sets of Hamiltonians without breaking TRS at any intermediate point. The trivial and nontrivial topological classes may be thought of as equivalence classes of Hamiltonians, which contain, respectively, members which display an even and an odd-quantized spin Hall conductance.

2. Three-dimensional insulators

The Brillouin zone for a 3D insulator has the topology of a 3D torus. We represent it by a cube \( \{-\pi \leq k_x, k_y, k_z \leq \pi \} \). Under the operation of the TRS operator, a Bloch wave function at point \( k \) gets mapped to point \(-k\). The plane in momentum space, \( k_z = 0 \), gets mapped onto...
itself under inversion and has the topology of a 2D torus. The spectral projector, \( P \), for the 3D insulator restricted to this plane, therefore, has an associated \( Z_2 \) invariant.

There are a number of such surfaces with which one may associate a \( Z_2 \) invariant. A few of these are the planes \( k_x = 0, k_x = \pi, k_y = 0, k_y = \pi, k_z = 0 \) and \( k_z = \pi \). The associated \( Z_2 \) invariants are denoted by \( v_1, v_2, \tilde{v}_2, v_3 \) and \( v_3 \), respectively. It was argued previously that the \( Z_2 \) invariants of these planes are not all independent [8]–[10]. The arguments were based on the counting of monopole charges [9], on contractions of the 3D EBZ to the 3D torus [8], or on the number of independent choices of time reversal polarizations [10]. Here, we provide a simple alternative argument for the number of independent \( Z_2 \) invariants in three dimensions. This argument also shows how the \( Z_2 \) invariants of planes such as \( k_x + k_y = 0 \) may be calculated from the other \( Z_2 \) invariants.

Consider the composite surface, \( S \), consisting of the shaded region in figure 1(a). This surface, which is a union of the two planes, \( k_y = 0 \) and \( k_z = \pi \), can be mapped onto a 2D torus and is mapped onto itself under inversion. Thus, a \( Z_2 \) invariant may be associated with this surface. The projection operator for this surface can be written in terms of the two projection operators as

\[
P = P' \oplus P'',
\]

where \( P' \) is the projection operator restricted to the plane \( k_x = \pi \) and \( P'' \) is restricted to the plane \( k_y = 0 \). Here, if \( P' = \sum_{\alpha \in \Sigma} |\alpha\rangle\langle\alpha| \), \( P'' = \sum_{\alpha \in \Sigma'} |\alpha\rangle\langle\alpha| \), by \( P \oplus P' \), we mean \( \sum_{\alpha \in \Sigma \cup \Sigma'} |\alpha\rangle\langle\alpha| \).

\( P', P' \), and \( P'' \) can be decomposed as in equation (1), and corresponding \( Z_2 \) invariants, \( v(P') \) and \( v(P'') \), can be defined. The projection operator, \( P \), can be decomposed as in equation (1) and can be written as \( P = P_1 + P_2 \), where \( P_1 = P_1' \oplus P_1'' \) and \( P' = P_1' + P_2' \), etc; and we again assume that suitable \( P_1, P_1' \) and \( P_2'' \) can be defined, which satisfy the above equations and are globally smooth on their domains of definition so that the corresponding Chern numbers are well defined.

It follows that

\[
v(P) = v(P') + v(P'') = v_2 + \tilde{v}_3. \tag{2}
\]

Consider now a continuous deformation of the surface parameterized by a variable, \( t \), which varies from 0 to 1 such that at every point of the deformation, the surface \( S(t) \) gets mapped onto itself under inversion. \( S(0) \) corresponds to the surface previously denoted by \( S \). A possible value of \( S(t) \) for \( 0 < t < 1 \) is shown in figure 1(b). At \( t = 1 \), the surface \( S(t) \) becomes the surface shown in figure 1(c). This surface is the union of the planes \( k_y = \pi \) and \( k_z = 0 \). Under this transformation, the projection operator that becomes a continuous function of \( t \), \( P(t) \), also changes continuously and the \( Z_2 \) invariant therefore does not change. (Note, however, that we do not require that \( P_1(t, k) \) is a smooth function of \( t \).)

Thus, it follows that

\[
v(P(1)) = v(P(0)) = v(P). \tag{3}
\]

Further, since \( S(1) \) can be regarded as the union of the planes \( k_y = \pi \) and \( k_z = 0 \),

\[
v(P(1)) = \tilde{v}_2 + v_3. \tag{4}
\]

Thus, from equations (2)–(4), we conclude that

\[
v_2 - \tilde{v}_2 = v_3 - \tilde{v}_3.
\]
The shaded region, $S$, in (a) is the union of the planes $k_y = 0$ and $k_z = \pi$. This region can be continuously deformed into the shaded regions in (b) and into the union of the planes $k_y = \pi$ and $k_z = 0$ shown in (c).

The plane $k_z = k_y$ can also be obtained as a deformation of the surface in figure 1(b). Thus the $Z_2$ invariant of this plane is obtained as $\nu_2 + \nu_3$. Similarly, by deforming surfaces $S'$, which we define as the union of the planes $k_x = 0$ and $k_y = \pi$, and $S''$, which we define as the union of the planes $k_y = 0$ and $k_z = \pi$, it can easily be shown that

$$\nu_1 - \tilde{\nu}_1 = \nu_2 - \tilde{\nu}_2 = \nu_3 - \tilde{\nu}_3.$$  

Further, the $Z_2$ invariant of any other plane that maps onto itself under TRS can also be obtained from the values of $\nu_1$, $\nu_2$, $\nu_3$ and $\nu_1 - \tilde{\nu}_1$. We can thus characterize any topological insulator with TRS in three dimensions with four invariants, which may be chosen to be $\nu_1$, $\nu_2$, $\nu_3$ and $|\nu_1 - \tilde{\nu}_1|$.

The arguments in [9] may be summarized as follows. The spectral projection operator in 3D when restricted to the planes $k_i = 0, k_i = \pi$ for $k_i \in \{k_x, k_y, k_z\}$ can be written as a sum $P = P_1 + P_2$, where $P_1$ and $P_2$ map onto each other under TRS.

Consider the set of momentum space slices, $k_z = c$, where $0 \leq c \leq \pi$. Let $P_1(c)$ and $P_2(c)$ be the restrictions of the operators $P_1$ and $P_2$ to the plane $k_z = c$. For an arbitrary value of $c$, these operators do not map onto each other under TRS. The $Z_2$ invariant is therefore not well defined in general. When the $Z_2$ invariants for the planes $k_z = 0$ and $k_z = \pi$ are different, the operators $P_1(0)$ and $P_1(\pi)$ have different Chern numbers. A continuous deformation of a 2D projection operator to one which has a different Chern number is not possible. Changes in Chern number may be regarded as occurring at singular diabolical points or monopoles at which the projection operator is not well defined. In general, one may define 2D surfaces enclosing points at which the projection operators $P_1$ and $P_2$ are not well defined and associate a charge with these surfaces. If the difference in the Chern number of $P_1$ on the slice $k_z = 0$ to the Chern number

\[ \nu_1 - \tilde{\nu}_1 \]
of $P_1$ on the slice $k_z = \pi$ is an odd integer, this implies the existence of a net odd monopole charge between these two planes and ensures that the $Z_2$ invariants of the planes $k_z = 0$ and $k_z = \pi$ are different. By a careful counting of monopole charges and by using TRS, one can then show that in this case, the $Z_2$ invariants of the $k_z = 0$ and $\pi$ planes also differ from each other and the same is true for the $k_y = 0$ and $\pi$ planes.

The fourth $Z_2$ invariant, $\nu_1 - \tilde{\nu}_1$, is an intrinsically 3D characteristic of the insulator. Insulators whose fourth $Z_2$ invariant is zero and one have been christened ‘weak’ and ‘strong’ topological insulators respectively. The existence of four independent invariants agrees with the results of [8] and [10]. The invariants there were obtained by contractions of the 3D EBZ to the three torus [8] and by counting the number of independent choices of the time reversal polarizations [10].

In summary, we have analyzed the Chern number formula for the $Z_2$ invariant in two dimensions. The trivial and nontrivial topological classes may be thought of as equivalence classes of Hamiltonians, which contain members with an even and an odd-quantized spin Hall conductance, respectively. A simple counting argument for the number of invariants in 3D was provided using deformations of planes that map onto themselves under time reversal.

Acknowledgments

I am grateful to John Chalker, Dmitry Kovrizhin and Steven Simon for useful discussions and comments on previous versions of this manuscript and acknowledge support from EPSRC grant EP/D050952/1.

References

[1] Klitzing K V, Dorda G and Pepper M 1980 Phys. Rev. Lett. 45 494
[2] Laughlin R B 1981 Phys. Rev. B 23 5632
[3] Thouless D J, Kohmoto M, Nightingale M P and den Nijs M 1982 Phys. Rev. Lett. 49 405
[4] Halperin B I 1982 Phys. Rev. B 25 2185
[5] Haldane F D M 1988 Phys. Rev. Lett. 61 2015
[6] Hatsugai Y 1993 Phys. Rev. Lett. 71 3697
[7] Kane C L and Mele E J 2005 Phys. Rev. Lett. 95 146802
[8] Moore J E and Balents L 2007 Phys. Rev. B 75 121306
[9] Roy R 2009 Phys. Rev. B 79 195322
[10] Fu L, Kane C L and Mele E J 2007 Phys. Rev. Lett. 98 106803
[11] Bernevig B A, Hughes T L and Zhang S 2006 Science 314 1757
[12] Konig M et al 2007 Science 318 766
[13] Fu L and Kane C L 2007 Phys. Rev. B 76 45302
[14] Hsieh D et al 2008 Nature 452 970
[15] Murakami S and Kuga S 2008 Phys. Rev. B 78 165313
[16] Qi X-L, Hughes T L and Zhang S-C 2008 Phys. Rev. B 78 195424
[17] Roy R 2009 Phys. Rev. B 79 195321
[18] Fu L and Kane C L 2006 Phys. Rev. B 74 195312
[19] Fukui T and Hatsugai Y 2007 J. Phys. Soc. Japan 76 053702
[20] Avron J E, Seiler R and Simon B 1983 Phys. Rev. Lett. 51 51
[21] Prodan E 2009 Phys. Rev. B 80 125327
[22] Sheng D N, Weng Z Y, Sheng L and Haldane F D M 2006 Phys. Rev. Lett. 97 036808