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Z_2 classification of quantum spin Hall systems: An approach using time-reversal invariance

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We study the phases of Bloch insulators with time-reversal symmetry on the basis of the homotopy of the ground-state wave functions in momentum space and find that there are two topological classes characterized by a Z_2 invariant. The results are in agreement with a recent study based on counting the zeroes of a certain Pfaffian function related to the ground-state wave function. It is shown that there is a link between the formulation of the topological invariant presented here and the number of robust edge states. A formula is also provided which greatly simplifies the computation of the invariant in a large number of cases. The present study provides guidance for the search of systems which belong to the nontrivial topological class and also establishes a link between the quantum spin Hall effect and the integer quantum Hall effect.

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I. INTRODUCTION

There has been a fair amount of recent theoretical and experimental interest in those transport properties of materials which involve the spin rather than the charge degree of freedom, fueled in part by the possibilities of their applications in devices. One of the more interesting phenomena that has been investigated is the spin Hall effect,[1,2] a phenomenon in which a spin current is generated in a transverse direction to an applied electric field. Recently, a number of two-dimensional (2D) models have been proposed where the quantum spin Hall effect (QSHE) is said to occur[3,4] In these models the spin Hall conductance, defined as the ratio of the spin-current density to the external electric field, is a multiple of e^2/h. This is reminiscent of the integer quantum Hall effect (IQHE) where the Hall conductance σ_{xy} is quantized: $\sigma_{xy}=ne^2/h$, where n is an integer. In the IQHE, systems with different values of n (where $\sigma_{xy}=ne^2/h$) belong to different phases, each of which is characterized by a topological invariant[5] whose value is n. The number n is also equal to the number of robust edge states in the system.[6,7]

In systems with time-reversal (TR) symmetry, no net charge currents can flow along the edges of the sample. However, pairs of edge channels which carry charge in opposite direction can still exist and are in fact a feature of some of the proposed models. Further, it has been noticed that there is a distinction between models with an odd number of pairs of zero-energy edge states and those with an even number of pairs of such edge states. An odd number of pairs of zero-energy edge states are stable against small TR invariant perturbations, while an even number of pairs is not.[8,9]

In the QSHE, the value of the spin Hall conductance is not quantized in general.[10] Thus, unlike the IQHE, the spin conductance cannot be used to classify different phases. However, a topological Z_2 invariant which takes only the values 0 and 1 has been introduced to characterize systems which display the QSHE, and more generally, any 2D Bloch insulator which preserves time-reversal symmetry.[11] This invariant is expressed in terms of the zeroes of a Pfaffian, and in this form, it is quite different from the topological invariant for the IQHE.

We thus see that there are two types of classification, one based on the number of robust edge states and another based on topology. It seems likely that these two classification schemes are related. Since a connection between the edge states and the topological invariant is well known in the case of the IQHE, establishing this link in the QSHE can lead to a deeper understanding of the relation between the IQHE and the QSHE. Establishing such a connection is therefore highly desirable and is one of the aims of this paper.

We present a formulation of the topological invariant which is based on the obstructions to continuing the wave functions in momentum space. We first consider a two-band model and study the topology of the wave functions in momentum space. We then generalize this to systems with an arbitrary number of band pairs. This formulation has several useful features. For instance, it makes it easy to compute the Z_2 invariant for a large number of models. It also provides guidance for the construction of models with a nontrivial Z_2 invariant besides providing a natural connection between the IQHE and the QSHE.

II. TOPOLOGY OF GROUND-STATE WAVE FUNCTIONS

A. Single pair of occupied bands

We first consider an insulator model which has a single pair of occupied bands in the ground state before generalizing our results to systems with an arbitrary even number of occupied bands. Since we only consider systems with time-reversal symmetric ground states, the number of occupied bands is always even. A generic four-band time-reversal-invariant tight-binding Hamiltonian can be written in momentum space in the form[11]

$$H(\boldsymbol{k}) = \sum_{a=1}^{5} d_a(\boldsymbol{k})\Gamma_a + \sum_{a<b=1}^{5} d_{ab}(\boldsymbol{k})\Gamma_{ab}, \tag{1}$$

where Γ_a's are the Dirac matrices as defined in Ref. 11 and the d_a's and d_{ab}'s are symmetric and antisymmetric functions in momentum space as required by time-reversal invariance. The ground state then consists of two bands which map onto each other under time reversal.

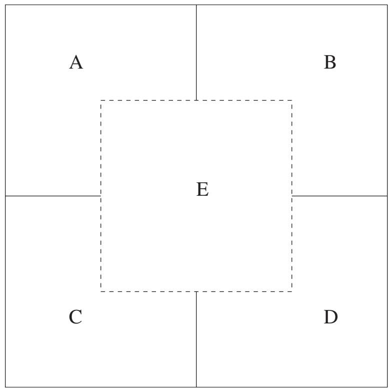

FIG. 1. The two-dimensional torus divided into five regions A, B, C, D, and E. The dashed curve marks the path along which we study the transition matrices.

Our approach will be to study the topology of the ground-state wave function which is closely related to the topology of the Bloch wave functions in momentum space. Momentum space is topologically equivalent to the two torus in this case. We will see that it is impossible to find a continuous set of Bloch wave functions which satisfy certain conditions that we will specify. This situation is analogous to the problem that arises in the specification of the wave function of an electron in the vicinity of a magnetic monopole (the so-called Dirac monopole). Consider the wave function of the electron on the surface of a two-dimensional sphere which surrounds a magnetic monopole. It is well known that the wave function cannot be continuously specified on the entire surface of the sphere. However two sets of continuous-wave functions can be found for the two hemispheres and these can be glued together. The difference in our case is that we have a two-dimensional spinor rather than a single-component wave function.

Let $V(\boldsymbol{k})$ be the vector space spanned by the two occupied bands at the point $\boldsymbol{k}$. Time-reversal symmetry leads to an involution on the torus and on the fiber bundle, i.e., it relates the wave functions at $\boldsymbol{k}$ to those at $-\boldsymbol{k}$. It is always possible to find locally continuous-wave functions in momentum space which span the vector space $V(\boldsymbol{k})$. However finding a globally continuous basis may not be possible. In such a case one can still construct locally continuous-wave functions and "glue" them together.[12] The topology of the Brillouin zone for a two-dimensional periodic lattice is equivalent to a two-dimensional torus. Consider a two-dimensional torus which we divide into five nonoverlapping regions A, B, C, D, and E as shown in Fig. 1. We also use the letters A, B, C, D, and E to denote open sets which contain and are slightly larger than the regions marked by these names in the figure, and E' to label the open set which contains the complement the region bounded by the dashed line. We study the transition matrices in the overlaps of these open sets.[13]

In the present case, it is sufficient to study the set of vector bundles which are homotopic to the one whose transition matrices across regions, A,B etc. differs from the identity only along the dashed line marked in the figure. This is equivalent to taking into consideration only those sets of wave functions which are locally continuous in E and E' (but not necessarily globally continuous). We consider a set of continuous orthogonal vector functions and define the basis vectors $(1,0)^T$ and $(0,1)^T$ in terms of these wave functions on the two regions separated by the dashed curve (namely the region E and its complement). These wave functions used as the basis for the vector space, $V(\boldsymbol{k})$, are chosen such that the following holds. If a wave function $\psi(\boldsymbol{k})$ is represented as $(v,\boldsymbol{k})$, where v is a spinor in the basis described above, then the operation of time reversal maps this onto the wave function which can be written in the same basis and representation as $[i\sigma_2 K_0(v),\Phi(\boldsymbol{k})]$, where Φ takes $\boldsymbol{k}$ to $-\boldsymbol{k}$, σ_2 is the Pauli sigma matrix, and K_0 is the operator which corresponds to complex conjugation.

We parametrize the dashed curve in Fig. 1 by the angle $\phi \in S^1$ (where S^1 is the unit circle) which varies from 0 to 2π in such a way that if the parameter ϕ corresponds to a point $\boldsymbol{k}$, then $\phi+\pi$ corresponds to the point $-\boldsymbol{k}$. If v and v' are two spinors which represent the same vector $\boldsymbol{v}$ at the point parametrized by ϕ in the two regions, E and E', then they are related by means of a transition matrix $v=U(\phi)v'$, where $U(\phi)\in \mathrm{U}(2)$. Here $\boldsymbol{v}$ is an element of $V(\phi)$ and is therefore an (arbitrary) linear combination of the energy eigenstates at the point ϕ. If we now write down the transition matrix $U(\phi)\in \mathrm{U}(2)$ for some value of ϕ in the form $e^{i\alpha I}e^{i\boldsymbol{n}.\boldsymbol{\sigma}\omega}$, then time-reversal invariance leads to the condition that

$$U(\phi+\pi) = e^{-i\alpha I}e^{i\boldsymbol{n}.\boldsymbol{\sigma}\omega}. \tag{2}$$

Here, σ_i are the Pauli sigma matrices.

It follows from Eq. (2) that if we write $U(\phi)$ as a function $e^{i\theta(\phi)I}g(\phi)$, where $\theta(\phi)$ and $g(\phi)\in \mathrm{SU}(2)$ are continuous functions, then these functions satisfy the conditions $\theta(\pi)=-\theta(0)+p\pi$, $g(\pi)=e^{-ip\pi I}g(0)$, where p is an integer. If p is even, $g(p)=g(0)$ and since $\pi_1[\mathrm{SU}(2)]=0$, it follows that the transition function in this case can be continuously deformed to the constant function $U(\phi)=e^{ip\pi/2}g(0)$. When p is odd, then $g(\pi)=-g(0)$ and thus $g(\pi)$ and $g(0)$ are always distinct elements for any value of $g(0)$. We can deform an arbitrary function $g(\phi)$ which satisfies this condition to the particular one $e^{ip\pi/2}e^{i(\phi+\pi/2)\sigma_3}$. Thus the class of transition functions consists of two distinct topological classes. An adiabatic change in the Hamiltonian leads to a continuous change in the transition function and vice versa. Hence, it follows that there are two distinct topological classes of ground-state wave functions.

We note that the above arguments can also be intuitively understood as follows:[14] the two occupied Bloch bands may be regarded as two components of a two-dimensional Dirac spinor with an effective SU(2) degree of freedom [the U(1) degree of freedom is absent due to time-reversal symmetry] with the restriction that the element of SU(2) at $\boldsymbol{k}$ and $-\boldsymbol{k}$ map onto the same element of $\mathrm{SU}(2)/Z_2$. The index is then equivalent to the fundamental group of $\mathrm{SU}(2)/Z_2$ which is Z_2.

To make the connection with the TKNN invariant[5] and Chern numbers, let us first suppose that the bands have well-defined Chern numbers. In this case, one can choose the energy eigenstates as the continuous-wave functions which define the basis of the vector space $V(\boldsymbol{k})$ at each point $\boldsymbol{k}$ in momentum space. The transition function which corresponds to bands with Chern numbers $n,-n$ can be continuously deformed to the diagonal matrix with entries $e^{in(\phi+\pi)}, e^{-in\phi}$. It is readily verified that p may be taken to be $\pm n$. The connection between Chern numbers of bands and number of robust edge states previously made in the context of integer quantum Hall systems[7] can now be extended to systems with time-reversal symmetry. The set of time-reversal-invariant band insulators with two occupied bands then fall into two topologically distinct categories: (i) when the bands carry even Chern numbers, the ground state is topologically equivalent (i.e., may be adiabatically continued) to the state with no edge modes and (ii) when the bands carry odd Chern numbers, the ground state is topologically equivalent to the state that has a single pair of edge modes.

If the Bloch wave functions are not continuous and differentiable and therefore have no well-defined Chern numbers, then one may still use the formula after the following steps. Suitable linear combination of the energy eigenstates can be chosen as the basis of orthogonal continuous-wave functions on the patches E and E' in such a way that these new wave functions then have well-defined Chern numbers. This follows from the fact that the transition matrices at the boundary of E and E' can always be transformed to a diagonal form as shown earlier and is consistent with the "splitting principle."[15] Alternatively, one may adiabatically continue the Hamiltonian to one whose filled bands have well-defined Chern numbers. The Chern numbers of these wave functions (the eigenstates of the new Hamiltonian or the linear combinations with well-defined Chern numbers) may then be used to calculate the Z_2 invariant.[16] The new Hamiltonian then has either an odd or an even number of edge modes depending on the value of the topological invariant. Further, since an odd number of pairs of edge states is stable whereas an even number of such pairs is not[8,9] and cannot, therefore, change under an adiabatic transformation, we may argue that the original Hamiltonian has either a single pair of robust edge states or none depending on whether it is in the nontrivial or the trivial topological class.

We have thus established a one-to-one correspondence between the systems with a nontrivial topological invariant and those with a robust pair of edge states.

B. Multiple pairs of occupied bands

We now consider a system with $2N$ occupied bands where N is a positive integer. We choose a basis for the vector bundles in each region chosen again such that the time-reversal operator in this basis is $JK_0\Phi$ in the notation used earlier where J is the matrix whose only nonzero elements are $J(2i,2i+1)=-J(2i+1,2i)=1$ and K_0 is the complex-conjugation operator as before. We write the transition function in the form $U(\phi)=e^{i\theta(\phi)}g(\phi)$, where $\theta(\phi)$ and $g(\phi)$ are continuous functions. Time-reversal invariance then leads to the conditions

$$\theta(\pi) = -\theta(0) + \frac{p\pi}{N}, \quad g(\pi) = e^{-ip\pi I/N} J g^*(0) J^{-1}. \tag{3}$$

In this case too there are two classes of transition functions corresponding to two classes of band structures depending on whether p is odd or even.

Since $\pi_1[\mathrm{SU}(2N)]=0$ we can continuously deform an arbitrary transition function $U(\phi)$ which satisfies the above constraints imposed by time-reversal invariance to one whose value at $\phi=0$ is the diagonal matrix with matrix elements $U[2i,2i]=e^{i\theta}e^{-i\alpha_i}e^{i\omega_i}$ and $U[2i+1,2i+1]=e^{i\theta}e^{i\alpha_i}e^{i\omega_i}$, where

$$\theta = \frac{p\pi}{2N},$$

$$\omega_i = \frac{-p\pi}{2N}, \quad i \neq 1,$$

$$\omega_1 = \frac{-\pi}{4} + (-1)^r\frac{\pi}{4} - \frac{p\pi}{2N},$$

$$\alpha_i = 0, \quad i \neq 1$$

$$\alpha_1 = \frac{\pi}{4} - (-1)^r\frac{\pi}{4}.$$

Here $r=p \bmod 2$.

If p is even, then $g(\pi)=g(0)$ and the transition function can be continuously deformed to a constant function. When p is odd, it can be easily shown that there is no $g(0)$ (not just diagonal) such that $g(\pi)=g(0)$. In this case it can be seen that a constant multiple of the matrix whose only nonzero elements are $U(\phi)[1,1]=e^{i\phi}$; $U(\phi)[2,2]=e^{-i(\phi+\pi)}$; $U(\phi)[i,i]=1, i\neq 1,2$ satisfies the condition at $\phi=0$ specified above.

It is easy to verify that if the bands have Chern numbers $\{c_i,-c_i\}$, then p may be taken to be $p=\Sigma_i c_i$.[17]

Let us define

$$C = \sum_{c_n>0} c_n, \tag{4}$$

where n is the band index[18] and c_n is the corresponding Chern number given by[19]

$$c_n = (i/2\pi)\int \mathrm{Tr}(dP_nP_ndP_n), \tag{5}$$

where $P_n(k)=|\psi_n(k)\rangle\langle\psi_n(k)|$ is the projection operator corresponding to the nth band. The sum is taken over the set of bands which have positive Chern numbers. Then we are led to define the Z_2 index

$$E = C \bmod 2, \tag{6}$$

which labels the topologically distinct classes of bands.

III. DISCUSSION

These results can also be understood from a band-touching picture. Time-reversal invariance dictates that when time-reversed pairs of bands touch, they do so at an even number of points and the Chern number exchange is always an even number. However, two sets of such bands, each with Chern numbers ± 1, may touch. The Chern number of each band after the exchange is zero.

Using the above formula, the Z_2 index of several recent quantum spin Hall models can be readily calculated. The index is equal to 1 for the models proposed in Refs. 2, 3, and 20. The Kane Mele Hamiltonian[3] for the spin Hall effect in graphene is equivalent to two copies of the Haldane Hamiltonian for the integer quantum Hall effect on a honeycomb lattice. Hence, the Chern numbers of the occupied bands are ± 1 in the quantum spin Hall phase. Hence, the invariant as calculated by the above formula is $E=1$. In the normal insulator phase, the Chern number of both the bands is zero, and hence $E=0$. These systems thus exhibit a topologically nontrivial phase and have robust edge states in certain phases.

The extension of the TKNN (Ref. 5) numbers to systems with interactions and disorder is usually done by expressing the Hall conductance of the bands in terms of the Chern numbers in the space of the parameters that determine generalized periodic boundary conditions. A spin-Chern number has been recently proposed by extending this idea to spin quantum Hall systems.[21] Our analysis suggests that while this classification is useful for the case when the Hamiltonian of the system can be derived from a Hamiltonian which has a pair of occupied bands whose Chern numbers are ± 1 in the ground state (with the rest of the occupied bands having zero Chern number), it might fail when this condition is not met.

The Z_2 index as formulated here and in Ref. 11 both provide a topological classification of band insulators in two dimensions. It follows from topological considerations of K theory[22] that they must be formally equivalent.

We have presented a Z_2 index, which has the advantage of being easy to compute in many cases, to characterize quantum spin Hall models and other time-reversal-invariant Bloch Hamiltonians. It is expressed in terms of the Chern numbers of the bands of the model, which leads to a link between the index and the number of pairs of robust edge states of the system. On the basis of K theory, an equivalence between the present index and the one presented by Kane and Mele is claimed. The invariance of the index was proved using topological obstruction arguments as well as a more intuitive band-touching argument. This study also suggests that the Z_2 index can be used to study other systems and leads to a natural connection between the quantum spin Hall effect and the integer quantum Hall effect. A method has recently been proposed which aids in the efficient calculation of the topological Z_2 index based on the obstruction method and the formula in terms of the Chern numbers presented above.[23]

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[15] See, for instance, page 383 of Ref. 24.
[16] Our analysis is therefore restricted to Hamiltonians which can be adiabatically continued to one whose filled bands have well-defined Chern numbers.
[17] In the case when the bands do not have well-defined Chern numbers, one may proceed by taking orthogonal linear combinations of them as in the case of a single pair of occupied bands.
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