Quantum Spin Hall Effect in Three Dimensional Materials: Lattice Computation of $Z_2$ Topological Invariants and Its Application to Bi and Sb

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We derive an efficient formula for $Z_2$ topological invariants characterizing the quantum spin Hall effect. It is defined in a lattice Brillouin zone, which enables us to implement numerical calculations for realistic models even in three dimensions. Based on this, we study the quantum spin Hall effect in Bi and Sb in quasi-two and three dimensions using a tight-binding model.

KEYWORDS: Quantum spin Hall effect, Time reversal symmetry, $Z_2$ topological invariant, Chern number, Lattice gauge theory

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Quantum spin Hall (QSH) effect$^{1-5}$ has been attracting much current interest as a new device of spintronics.$^{6,8}$ It is a topological insulator$^{10-12}$ analogous to the quantum Hall (QH) effect, but it is realized in time-reversal ($T$) invariant systems. While QH states are specified by Chern numbers,$^{13,14}$ QSH states are characterized by $Z_2$ topological numbers,$^2$ which suggests that $Z_2$ invariants would have deep relationship with the $Z_2$ anomaly of the Majorana fermions.$^{15,16}$

Graphene has been expected to be in the QSH phase.$^{1,2}$ However, recent calculations have suggested that the spin-orbit coupling in graphene is too small to reveal the QSH effect experimentally.$^{17,18}$ Recently, it has been pointed out that Bi thin film is another plausible material for QSH effect.$^{19}$ Also by the idea of adiabatic deformation of the diamond lattice, it has been conjectured that Bi in three dimensions (3D) is in a topological phase.$^{20}$

While systems in two dimensions (2D) are characterized by a single $Z_2$ topological invariant, four independent $Z_2$ invariants are needed in 3D.$^{20-23}$ This makes it difficult to investigate realistic models, in which complicated many-band structure is involved. Therefore, for the direct study of Bi in 3D as well as for the search for other materials, to establish a simple and efficient computational method of $Z_2$ invariants in 3D is an urgent issue to be resolved.

In this paper, we present a method of computing $Z_2$ invariants based on the formula derived by Fu and Kane$^{24}$ together with the recent development of computing Chern numbers in a lattice Brillouin zone.$^{25-27}$ This method is based on recent developments in lattice gauge theories$^{30-35}$ but simple enough to compute $Z_2$ invariants even for realistic 3D systems. Based on this, we study a tight-binding model for Bi and Sb.

First, we derive a lattice version of the Fu–Kane formula.$^{24}$ To this end, we restrict our discussions, for simplicity, to systems in 2D, where a single $Z_2$ invariant is relevant. Let $T$ be the time-reversal transformation $T = i\sigma^2 K$, and assume that the Hamiltonian in the momentum space $\mathcal{H}(k)$ transforms under $T$ as $\mathcal{T} \mathcal{H}(k) T^{-1} = \mathcal{H}(-k)$. Let $\psi(k) = (|1(k)\rangle, \ldots, |2M(k)\rangle)$ denote the $2M$ dimensional ground state multiplet of the Hamiltonian: $\mathcal{H}(k)|n(k)\rangle = E_n(k)|n(k)\rangle$.$^{11,12}$ Assuming that the many-body energy gap is finite, we focus on topological invariants under the $U(2M)$ transformation

$$\psi(k) \rightarrow \psi(k) U(k), \quad U(k) \in U(2M).$$

(1)

As discussed,$^{22,27}$ the pfaffian defined by $p(k) = pf \Psi^\dagger(T \Psi)$ characterizes the topological phases of $T$ invariant systems. To be precise, the systems belong to topological insulator if the number of zeros of the pfaffian in half the Brillouin zone is 1 (mod 2), and belong to simple insulator otherwise. This number has been referred to as $Z_2$ invariant. It should be noted that under eq. (1), the pfaffian $p(k)$ transforms as $p(k) \rightarrow e^{-i\phi(k)} p(k)$, where $\phi(k)$ is the $U(1)$ part of $U(2M)$ defined through the relation $e^{i\phi(k)} \equiv det U(k)$.

Recently, Fu and Kane$^{24}$ have shown that the $Z_2$ invariant is expressed alternatively by

$$D = \frac{1}{2\pi i} \left[ \oint_{\partial B^-} A - \int_{B^-} F \right],$$

(2)

where $B^- = [-\pi, \pi] \otimes [-\pi, 0]$ (see Fig. 1), and where $A$ and $F$ is, respectively, the Berry gauge potential and associated field strength defined by $A = Tr \psi^\dagger d\psi$ and $F = dA$. Notice that the gauge transformation (1) yields $A \rightarrow A + id\phi$. This implies that the gauge of the Berry gauge potential can be fixed by the condition that the pfaffian

Fig. 1. (Color online) Left: The Brillouin zone, where shaded region denotes $B^-$. The thick lines indicate the boundary of $B^-$. The integration over $C_2$ gives a winding number. Right: A lattice on the Brillouin zone. The sites in $B_+^\ast$, $B_-^\ast$, and $B_0^\ast$ are denoted by blue, red, and black circles, respectively. The shaded region denotes the plaquettes in $B^-$. 

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p(k) is real positive. Note also that A(−k) = A(k) holds in this
gauge. This is a kind of T constraint, as stressed by Fu
and Kane.24) The zeros of p(k) thus serve as an obstruction of
the gauge fixing.28)
In systems with breaking T symmetry like QH effect,
such an obstruction gives in general a nontrivial Chern
number. Contrary to this, in systems under consideration, the
Chern number always vanishes due to T invariance. Even in
this case, an obstruction occurs in the Brillouin zone as long
as the zeros of the pfaffian exist. Since the zeros occur at the
time reversed pairs of points ±k∗, the vortices around these
pairs are opposite and therefore cancel each other, giving
vanishing Chern number. Nevertheless the sum of vorticities
in half the Brillouin zone, e.g., in B+ , just gives the number
of zeros of p(k) (mod 2). (Example, for example, that two
zeros exist in B−. Since they are generically first order zeros,
the winding numbers are ±1. Then their sum is restricted to ±2
and 0, which can be denoted as “0 mod 2”. It thus turns out that the Fu–Kane formula (2) counts the vorticities in half
the Brillouin zone. So far we have discussed in a specific
gauge, but in any other gauge, D changes by 2, provided that
the gauge keeps T constraint. Therefore, D is indeed a Z2
topological invariant. It has also a topological stability against
small perturbation as long as the many-body gap is finite. As we will show below, this expression for Z2 invariant is
convenient for numerical computations.
Define a lattice on the Brillouin zone,

\[ \mathbf{k}_i = (t_1/N_1, t_2/N_2), \quad j_{\mu} = -N_{\mu}, \ldots, N_{\mu}. \]  

(3)
The sites labeled by \( \mathbf{k}_i \) are divided into three sets, \( B^+ \) and T
invariant sites \( B^0 \) denoted by red, blue and black circles in
Fig. 1, respectively. Here, T invariant sites are specified by
the property that \( T \mathbf{H}(\mathbf{k}_i) T^{-1} = \mathbf{H}(\mathbf{k}_i) \). As a T constraint, we
choose the states at \( -\mathbf{k}_i \in B^0 \) as their Kramers doublets at
\( \mathbf{k}_i \in B^- \). Suppose that at \( \mathbf{k}_i \) the spectrum is arranged as
\( \epsilon_\mathbf{n}(\mathbf{k}_i) \leq \epsilon_{n+1}(\mathbf{k}_i) \). Then the states at \( -\mathbf{k}_i \) can be constrained as

\[ |n(-\mathbf{k}_i)\rangle = T|n(\mathbf{k}_i)\rangle, \quad \text{for} \quad \mathbf{k}_i \in B^- \].

(4)
On the other hand, both of the Kramers doublets are included
in \( B^0 \). The spectrum in this set can be arranged in general as
\( \epsilon_{2n}(\mathbf{k}) \leq \epsilon_{2n+1}(\mathbf{k}) \). Therefore, we enforce the constraint

\[ |2n(\mathbf{k}_i)\rangle = T|2n-1(\mathbf{k}_i)\rangle, \quad \text{for} \quad \mathbf{k}_i \in B^0 \].

(5)
With these constrained states, we define a link variable

\[ U_{\mu}(\mathbf{k}_i) = N^{-1}_{\mu}(\mathbf{k}_i) \psi^\dagger(\mathbf{k}_i) \psi(\mathbf{k}_i + \mu), \]

(6)
where \( N_{\mu}(\mathbf{k}_i) = |\psi^\dagger(\mathbf{k}_i) \psi(\mathbf{k}_i + \mu)\rangle \), and associated field
strength through a plaquette variable

\[ F_{12}(\mathbf{k}_i) = \text{Im} U_{12}(\mathbf{k}_i) U_{21}^{-1}(\mathbf{k}_i) = \text{Im} U_{12}(\mathbf{k}_i) U_{21}^{-1}(\mathbf{k}_i), \]

(7)
where \( F_{12} \) is defined within the branch \( F_{12}/i = (-\pi, \pi) \).

The sum of \( F_{12} \) over \( B^- \) can be written as a similar
formula to eq. (2). To see this, it is convenient to define a
gauge potential via \( A_{\mu}(\mathbf{k}_i) = \text{Im} U_{\mu}(\mathbf{k}_i) \) also in the branch
\( A_{\mu}(\mathbf{k}_i)/i = (-\pi, \pi) \). Then the field strength can be rewritten as

\[ F_{12}(\mathbf{k}_i) = \Delta_{1} A_{2}(\mathbf{k}_i) - \Delta_{2} A_{1}(\mathbf{k}_i) + 2\pi n_{12}(\mathbf{k}_i), \]

(8)
where integral field \( n_{12}(\mathbf{k}_i) \) has been introduced so as to
match the branches of both sides.\(^{25,34,35}\) Thus, we reach

\[ \sum_{\mathbf{k}_i \in B^-} F_{12}(\mathbf{k}_i) = \sum_{\mathbf{k}_i \in B^-} A_{1}(\mathbf{k}_i) + 2\pi \sum_{\mathbf{k}_i \in B^-} n_{12}(\mathbf{k}_i), \]

(9)
where the sums of \( F_{12} \) and of \( n_{12} \) are over the plaquettes
in the shaded region denoted by \( B^- \) in Fig. 1. The sum of \( A_{\mu} \)
is over the links of the boundary of \( B^- \) specified by thick
lines in Fig. 1. Therefore, a lattice version of \( D \) is

\[ D_L = \frac{1}{2\pi} \left[ \sum_{\mathbf{k}_i \in B^-} A_{1}(\mathbf{k}_i) - \sum_{\mathbf{k}_i \in B^-} F_{12}(\mathbf{k}_i) \right] \]

\[ = -\sum_{\mathbf{k}_i \in B^-} n_{12}(\mathbf{k}_i). \]

(10)
This formula for the Z2 invariants is one of the main results
of this paper. Indeed this formula has the following desired
properties. Firstly, it is strictly integral. Secondly, though
the ground state multiplet can be mixed by eq. (1), it is SU(2M)
invariant. Finally, it changes by 2 under the remaining U(1)
transformation, and hence, it is Z2 invariant. The last
property will be proved elsewhere, though it is not difficult.
In 3D, it has been shown that the phases of T invariant
systems are classified by four independent Z2 invariants.\(^{20-22}\)
To compute them, let us define six two-dimensional
tori, according to Moore and Balents.\(^{21}\) For example, fix
the third momentum to \( k_z = 0 \) or \( \pi \), then we have two tori
spanned by \( k_1 \) and \( k_2 \) which we denote \( Z_0 \) and \( Z_\pi \) torus,
respectively. Applying the previous techniques, we can compute two Z2 invariants \( D_L \) which are referred to as \( Z_0 \)
and \( Z_\pi \). In the same way, we have six invariants \( X_0, X_\pi, Y_0, Y_\pi, Z_0, \) and \( Z_\pi \) living on six tori \( X_0, X_\pi, Y_0, Y_\pi, Z_0, \) and \( Z_\pi \),
respectively. There are two constraints, however: \( x_0 x_3 = y_0 y_3 = z_0 z_3 \) (mod 2), and therefore, four invariants among
six are independent.\(^{21}\) According to Fu et al.,\(^{20}\) we choose
them as \( v_0 = x_0 x_3, \quad v_1 = x_0, \quad v_2 = y_0, \) and \( v_3 = z_3 \),
and denote them as \( v_{12}(11) v_{13}(12) \). As is known in the QH effects,
non-trivial structures of topological ordered states are hidden
in the bulk and play physical roles near the boundaries as
characteristic edge states.\(^{29}\) Based on the principle, by
investigating the relationship between the Z2 invariants and
surface states, Fu et al. have clarified that there are basically
three phases; simple band insulator, weak topological
insulator (WTI) which is topological but weak against
disorder, and more robust strong topological insulator
(STI).\(^{20}\)
Recently, Murakami\(^{39}\) has pointed out the possibility of
QSH effect in Bi. Though Bi is a semimetal, the valence
band and conduction band keep the direct gap throughout
the Brillouin zone. Fu et al. have studied solvable tight-binding
models with the diamond structure, and predicted that the
valence band of Bi is characterized by the WTI phase
specified \( \mathbf{0} = (111) \), based on the observation that the structure
of Bi can be viewed as an adiabatically distorted cubic
lattice toward the diamond lattice. However, since a realistic
tight-binding model including s and p orbitals with nearest
neighbor, second neighbor, and third neighbor hoppings
has indeed complicated band structure, we calculate the Z2
invariants directly for heavy group V elements.
In what follows, we investigate real materials by the tight-
binding models in ref. 36. We first discuss the phase of Bi
which is attracting much interest. We show in Fig. 2 examples of the $n$-field configuration computed for Bi. Though these calculations are for rather coarse $10 \times 10$ lattice, we have checked that finer ones indeed reproduce the same $Z_2$ invariants and our formula is actually convergent even in this mesh size. For Bi, these figures tell that $z_0 = 2$ and $z_n = 0$ for Bi, and $z_0 = 0$ and $z_n = 1$ for Sb.

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On the other hand, decreasing the thickness, a semimetal–semiconductor transition occurs, and Murakami has suggested that Bi thin film would be in QSH phase. To study the quasi 2D systems, and also to clarify the discrepancy between our result and the conjecture by Fu et al., we next investigate the effects of dimensionality on the present
model. We replace the Slater–Koster parameters $V_a$ ($a = ssa, sp\sigma, p\sigma\sigma, p\pi\pi$) for second neighbor hopping in ref. 36 by $fV_a$ with a uniform factor $f$. This factor $f$ can effectively control the dimensionality into [111] direction, interpolating between Murakami’s model at $f = 0$ and the 3D model at $f = 1$.

We show in Fig. 4 the band structure of Bi with $f = 0.5$ and 0.1. At $f = 1$ (see ref. 36), the overlap energy (indirect gap) is $\Delta E = -12\text{meV}$. With decreasing $f$, a semimetal–semiconductor transition occurs at $f \approx 0.99$. Figure 4 confirms that Bi is indeed a semiconductor at $f = 0.5$ and 0.1 whose overlap energy is $\Delta E = 56$ and 90 meV, respectively. Near $f = 0.993$, the phase of Bi changes from $0;(000)$ into $1;(111)$, At further decreasing $f$ and enhancing the two-dimensionality, topological change occurs again near $f \approx 0.223$, and the system becomes $0;(111)$, as shown in Fig. 5. This is just the phase predicted by Fu et al.\(^{20}\)

Therefore, we suggest that the adiabatic distortion of the diamond lattice leads to Bi thin film, and along the change of the dimensionality, the adiabatic distortion does not work, giving rise to gap-closing and resultant topological changes. We also conjecture that STI phase is very stable along the change of $f$, and could be observed by experiments.

Sb is also a semimetal with a larger gap at the $L$ point.\(^{36}\) We show in Fig. 3 the phase diagram of Sb. It turns out that Sb belongs to the $1;(111)$ phase even in 3D. Its location is far from the phase boundary with $0;(000)$ and therefore, it is rather stable. We show in Fig. 4 the band structure of Sb. With decreasing $f$, a semimetal–semiconductor transition also occurs at $f \approx 0.89$. Along the change of $f$, topological change occurs once: Near $f \approx 0.54$, the phase changes from $1;(111)$ into $0;(000)$, and no $0;(111)$ phase is observed throughout. Therefore, the phase of Sb thin film is $0;(000)$, different from Bi. In Fig. 5, we show the phase diagram of Sb for $f = 0.1$. However, it should be stressed that with appropriate thickness, $0.54 \leq f \leq 0.89$, Sb is a semiconductor in STI phase and hence should show QSH effect.

Finally, we comment on the relationship between the method presented in this paper and the previous one in ref. 27. While in the present calculation link variables are defined with respect to the momentum, the previous calculation has been implemented with respect to twist angles by imposing a spin-dependent twisted boundary condition. For systems with appropriate strength of spin–orbit coupling, the present computation is more efficient, but for systems with very small spin–orbit coupling as well as with inversion symmetry, the previous computation by the use of the twisted boundary condition gives more reliable results. In this sense, both methods are complementary to each other. Details will be published elsewhere.

We also mention that recently Fu and Kane\(^{37}\) have reached the similar conclusion of the phases of Bi and Sb by making the use of inversion symmetry of the system. We stress here that our method can apply to any systems, even without inversion symmetry.

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