Equivalent topological invariants of topological insulators

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Abstract. A time-reversal (TR) invariant topological insulator can be generally defined by the effective topological field theory with a quantized $\theta$ coefficient, which can only take values of 0 or $\pi$. This theory is generally valid for an arbitrarily interacting system and the quantization of the $\theta$ invariant can be directly measured experimentally. Reduced to the case of a non-interacting system, the $\theta$ invariant can be expressed as an integral over the entire three-dimensional Brillouin zone. Alternatively, non-interacting insulators can be classified by topological invariants defined over discrete TR invariant momenta. In this paper, we show the complete equivalence between the integral and the discrete invariants of the topological insulator.

Contents

1. Introduction 2
2. A pedagogical example 4
3. Equivalence between integral and discrete topological invariants 6
Acknowledgments 10
Appendix. Discussion on the global basis of wavefunctions 10
References 11
1. Introduction

In condensed matter systems, most states of matter are classified by the symmetries they break. For example, a crystal breaks the translational symmetry, a magnet breaks the rotational symmetry and a superconductor breaks the gauge symmetry. These broken symmetry states are identified by the order parameter, and described by the effective field theory. The effective field theory is constrained by the broken symmetry, and it defines universality classes of different states of matter, and predicts universal physical properties.

The quantum Hall (QH) state is a topological state of matter which does not fall into the conventional Landau paradigm. The long-distance and low-energy properties of the QH state we generally describe by the effective topological field theory

$$S_{\text{eff}} = \frac{C_1}{4\pi} \int \mathrm{d}^2 x \mathrm{d}t \epsilon^{\mu\nu\tau} A_\mu \partial_\nu A_\tau.$$  \hspace{1cm} (1)

This topological field theory is generally valid for interacting systems, and describes the electromagnetic response in the long wave length limit [1]. In the non-interacting limit, the Hall conductance $\sigma_{xy} = C_1$ can be expressed as a topological invariant over the two-dimensional (2D) Brillouin zone [2], given by

$$C_1 = \frac{e^2}{2\hbar} \int \mathrm{d}k_x \int \mathrm{d}k_y f_{xy}(k),$$  \hspace{1cm} (2)

where

$$f_{xy}(k) = \frac{\partial a_y(k)}{\partial k_x} - \frac{\partial a_x(k)}{\partial k_y},$$

$$a_i(k) = -i \sum_{\alpha \in \text{occ}} \langle \alpha k | \frac{\partial}{\partial k_i} | \alpha k \rangle, \hspace{1cm} i = x, y$$

are the Abelian Berry curvature and potential for the band states $|\alpha k\rangle$. Time-reversal (TR) symmetry breaking is essential for the QH effect.

More recently, new topological insulator states have been theoretically predicted and experimentally observed in HgTe quantum wells, BiSb alloys, and Bi$_2$Te$_3$ and Bi$_2$Se$_3$ crystals [3]–[9]. These topological insulator states physically arise from the spin–orbit coupling in electronic structures and are protected by the TR symmetry [5], [10]–[13]. A general theory describes the three-dimensional (3D) topological insulator in terms of an effective topological field theory [11], given by

$$S_{\text{eff}} = S_{\text{Maxwell}} + S_{\text{topo}} = \int \mathrm{d}^3 x \mathrm{d}t \left[ \frac{1}{16\pi} F_{\mu\nu} F^{\mu\nu} + \frac{\theta \alpha}{32\pi^2} \epsilon^{\mu\nu\sigma\tau} F_{\mu\nu} F_{\sigma\tau} \right]$$  \hspace{1cm} (3)

where the last term is the topological term and $\alpha = e^2/\hbar c$ is the fine-structure constant. For a period system, the partition function is invariant under the shift of $\theta$ by integer multiples of $2\pi$. Since TR transformation replaces $\theta$ by $-\theta$, only two special, quantized values of $\theta = 0$ and $\theta = \pi$ are consistent with the TR symmetry. Therefore, all TR invariant insulators fall into the two distinct classes, disconnected from each other. The Standard Model of elementary particles also admits such a topological term, therefore the study of the topological insulator can also shed light on the fundamental topological interactions in nature [14].

We can always couple an arbitrarily interacting electron system to the external electromagnetic field, and integrate out all the electronic degrees of freedom to obtain the
effective field theory (3). For a TR invariant insulator, only two discrete possibilities of \( \theta = 0 \) and \( \theta = \pi \) can be realized. For a non-interacting band insulator, Qi, Hughes and Zhang (QHZ) gave an explicit formula for the \( \theta \) parameter as an integral over the 3D Brillouin zone

\[
\theta \equiv 2\pi P_3(\theta) = \frac{1}{8\pi} \int d^3k e^{ijk} \text{tr}[\{f_{ij}(k) - \frac{2}{3}i a_i(k) \cdot a_j(k)\} \cdot a_k(k)]
\]

where

\[
f_{ij}^{\alpha\beta} = \partial_i a_{j}^{\alpha\beta} - \partial_j a_{i}^{\alpha\beta} + i [a_i, a_j]^{\alpha\beta},
\]

\[a_i^{\alpha\beta}(k) = -i \langle \alpha, k | \frac{\partial}{\partial k_i} | \beta, k \rangle
\]

are the non-Abelian Berry curvature and potential for the band state \( |\beta, k\rangle \). This topological invariant has the physical interpretation of a magneto-electric polarization, which can be directly measured experimentally [11, 15].

We notice a beautiful symmetry between the topological field theory of the TR breaking QH state and the TR invariant topological insulator state. Both the space-time integrals (1), (3) and the Brillouin zone integrals (2), (4) are integral topological invariants in the theory of differential geometry. We see that the TR breaking QH state is described by a Chern–Simons integral over the (2 + 1)-dimensional space-time (1), and a first Chern integral over the 2D Brillouin zone (2), while the TR invariant topological insulator is described by the second Chern integral over the (3 + 1)-dimensional space-time (3) and a Chern–Simons integral (4) over the 3D Brillouin zone. These are the deepest and most natural topological invariants in mathematics, and it is gratifying to see that they also describe topological states realized in nature.

TR invariant insulators form a universality class extending over the 4D, 3D and 2D space. The root state of this universality class is the topological insulator in 4D [16, 17]. In fact, it was the first TR invariant insulator state introduced theoretically, and historically it was referred to as the 4D QH state. It is described by a topological field theory

\[
S_{\text{eff}} = \frac{C_2}{24\pi^2} \int d^4x d\tau \epsilon^{\mu\nu\rho\sigma} A_{\mu} \partial_{\nu} A_{\rho} \partial_{\sigma} A_{\tau}.
\]

Under the TR transformation

\[A_0 \rightarrow A_0, \quad A_i \rightarrow -A_i
\]

therefore, we see that the topological field theory in (2 + 1) dimensions (1) breaks the TR symmetry, whereas the topological field theory in (4 + 1) dimensions (5) preserves the TR symmetry, and naturally describes the TR invariant topological insulators. For the case of non-interacting fermions, the coefficient is given explicitly by the second Chern number

\[
C_2 = \frac{1}{32\pi^2} \int d^4k e^{ijkkl} \text{tr} [f_{ij} f_{kl}].
\]

The TR invariant topological insulator defined by (5) and (7) in the 4D space naturally generalizes the corresponding quantities of the TR breaking topological insulator defined by (1) and (2) in the 2D space. This is why it was historically referred to as the 4D QH state [16, 17]. It is the root state for all TR invariant topological insulators in 3D and 2D, which can be obtained from the root state in 4D through the process of dimensional reduction [11].

Topological invariants in 3D band insulators have been studied from a different approach [12, 13]. In a series of beautiful papers, Fu, Kane and Mele (FKM) introduced a
Figure 1. Map between two circles $M$ and $N$. The arrows indicate the map. The winding number of (a), (b) and (c) is 1, 2 and 1, respectively.

$Z_2$ topological invariant [5, 12, 18] for the strong topological insulator, expressed as a discrete product over the eight TR invariant momenta (TRIM), explicitly written as

$$(-1)^{\nu_0} = \prod_{i=1}^{8} \delta_i,$$

where $\delta_i$ is quantity defined at TRIM $\Gamma_i$, the detailed form of which will be given in the following sections. Since weak topological insulators may not be generally robust, we will not be concerned with their definitions here.

Therefore, there are now two topological invariants defined for the topological insulator. They are motivated by different logical reasoning and have different mathematical forms. The integral invariant (4) given by QHZ is physically measurable in terms of the magneto-electric polarization, and leads directly to the general topological field theory (3). The discrete invariant (8) given by FKM has the distinct advantage that it can be easily evaluated, especially for crystals with inversion symmetry. Applied to concrete models of topological insulators [11, 19], these two definitions yield the same result. However, it is highly desirable to prove the general equivalence between these two definitions. In this paper, we show explicitly that one can transform the integral invariant (4) to the discrete invariant (8) exactly, proving the precise equivalence between these two definitions.

2. A pedagogical example

Because our approach involved the mathematical concept of degree of map, we shall give a brief introduction to it. Our presentation in this section is mainly designed for intuitive understanding, rather than mathematical rigor. Therefore, we shall illustrate the idea of degree of map in a simple one-dimensional example. For more mathematical details, see [20]. Those readers who are already familiar with this subject may omit this section.

Let us consider one concrete example. Consider a map $f : M \rightarrow N$, where $M$ and $N$ are both one-dimensional circles $S^1$ (see figure 1). The coordinates of $M$ and $N$ are denoted as $\phi$
and \( \theta \), respectively. The degree of map \( f \) is just the number of times that \( M \) covers \( N \) under \( f \) and it is often called the winding number.

The standard integral form of the winding number is defined as

\[
\deg(f) = \frac{1}{2\pi} \int_{\phi=0}^{\phi=2\pi} d\theta(\phi) = \frac{1}{2\pi} \int_{\phi=0}^{\phi=2\pi} \frac{d\theta}{d\phi} d\phi = n \in \mathbb{Z},
\]

which has a simple geometrical interpretation. For simplicity, let us assume that the point \( \phi = 0 \) maps to \( \theta = 0 \). When \( \phi \) goes from 0 to \( 2\pi \), \( \theta \) goes from 0 to \( 2\pi n \). This integral form of the winding number can be expressed in a discrete form. We arbitrarily choose an image point \( p \) on the image manifold \( N \) (see figure 1 for illustration), and count the number of source points \( \overline{p_1}, \overline{p_2}, \overline{p_3} \), etc on the source manifold \( M \), where the source points are weighted by the \( +1 \) or \( -1 \) sign depending on the orientation of the map. For example, image point \( q \) has only one source point \( \overline{q} \), which maps onto \( q \) in a clockwise sense. Therefore \( \deg(f) = 1 \). On the other hand, the image point \( p \) has three source points \( \overline{p_1}, \overline{p_2}, \overline{p_3} \), \( \overline{p_1} \) and \( \overline{p_2} \) map onto \( p \) in a clockwise sense, while \( \overline{p_2} \) maps onto \( p \) in a counterclockwise sense, giving \( \deg(f) = +1 - 1 + 1 = 1 \). We see from this example that the integral invariant of the winding number can be reduced to counting the weighted number of source points of a given image point—this is a discrete invariant for the winding number.

The above picture can be generalized to higher dimensions. Generally, for a map \( f : M \to N \), where \( M \) and \( N \) are both \( d \)-dimensional orientable manifold, we can define the degree of map as

\[
\deg(f) = \int_M f^*(\omega),
\]

where \( \omega \) is a \( d \)-form volume element on \( N \) satisfying \( \int_N \omega = 1 \), and \( f^*(\omega) \) is the pullback of \( \omega \) to \( M \) under \( f \). In our one-dimensional example discussed earlier, \( \omega = \frac{d\theta}{2\pi} \), and \( f^*(\omega) = \frac{d\theta}{d\phi} / 2\pi = \frac{(d\theta/d\phi) d\phi}{2\pi} \).

In our one-dimensional example, we have seen that there is a discrete form of the invariant \( \deg(f) \). This can also be generalized to higher dimensions. It is given as [20]

\[
\deg(f) = N[f^{-1}(p), J_{f^{-1}(p)} > 0] - N[f^{-1}(p), J_{f^{-1}(p)} < 0],
\]

where \( J \) is the Jacobian of the map, and \( N[f^{-1}(p), J_{f^{-1}(p)} > (\leq)0] \) denotes the number of source points mapping to \( p \) with a positive (negative) Jacobian, respectively. Without going into the general derivation of this formula, we just give the explanation in our one-dimensional example. In that example, \( J_{f^{-1}(p)} \) is the direction sense (clockwise or counterclockwise) of the map at the point \( p \), which is exactly what we have discussed earlier. We also mention that the point \( p \) in (11) should be regular, which means that the Jacobian of the map is nonzero at \( f^{-1}(p) \). Because the set of non-regular points has zero measure, we can always perturb the map to remove non-regularity at a given point.

In summary, we showed that the degree of a map can be expressed in two equivalent forms, the integral form (10) and the discrete form (11). In the next section, we will apply this idea to the integral and the discrete invariants of (4) and (8), which are degree of map \( \deg(f) \) modulo 2, simply denoted as \( \text{deg}_2(f) \).

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3. Equivalence between integral and discrete topological invariants

Let us start from the band structure of TR invariant topological insulators. To simplify the problem, we first assume that there are no degeneracies except those required by TR symmetry. Suppose that there are $2N$ filled bands labeled by $(\alpha, \beta, \ldots)$, where the number of filled bands is even because of the Kramers degeneracy. The $2N \times 2N$ matrix $B(k)$ is defined by

$$| -k, \alpha \rangle = \sum_\beta B_{\alpha \beta}^*(k) | \Theta, k, \beta \rangle,$$

(12)

where $| \Theta, k, \beta \rangle = \hat{\Theta} | k, \beta \rangle$ and $\hat{\Theta}$ is the TR operator. The property $\hat{\Theta}^2 = -1$ is crucial for TR invariant Fermi systems. By direct calculation we get the inner product

$$\langle -k, \alpha | \Theta, k, \beta \rangle = \sum_{\gamma} B_{\alpha \gamma}(k) \delta_{\gamma \beta},$$

(13)

and an important property of $B(k)$

$$B_{\alpha \beta}(-k) = \langle k, \alpha | \Theta, -k, \beta \rangle$$

$$= - \langle -k, \beta | \Theta, k, \alpha \rangle$$

$$= - B_{\beta \alpha}(k),$$

(14)

where the facts that $\hat{\Theta}^2 = -1$ and $\langle \alpha | \Theta, \beta \rangle = - \langle \beta | \Theta, \alpha \rangle$ have been used. Therefore, $B_{\alpha \beta}(-k)$ is antisymmetric at the eight TRIM, which enables the definition of the Pfaffian at these points. The definition of the discrete invariant given by FKM [12, 18] is expressed as

$$(-1)^{\nu_0} = \prod_{i=1}^{8} \delta_i; \quad \delta_i = \frac{\sqrt{\text{det}[B(\Gamma_i)]}}{\text{Pf}[B(\Gamma_i)]} = \pm 1$$

with the Pfaffian of $B$ written as Pf[$B$]. Although it seems that all the quantities appearing in this definition are local, global information on the Brillouin zone $T^3$(three-dimensional torus) is encoded because a global basis of wavefunction is required in this definition. The existence of the global basis is not obvious and we shall present a discussion on this in the appendix. The unitary matrix $B(k)$ defines a map

$$f : T^3 \rightarrow U(2N).$$

(15)

This map can be simplified since we have the assumption of absence of accidental degeneracies. We divide the $2N$ filled bands into $N$ TR pairs. Because energy eigenstates with different eigenenergy are orthogonal, we have $B_{\alpha \beta}(k) = 0$ if $| -k, \alpha \rangle$ and $| k, \beta \rangle$ belong to different pairs. Therefore, all the inter-pair elements of matrix $B(k)$ are zero. Written explicitly, the matrix $B(k)$ takes the following form

$$B(k) = \begin{bmatrix}
B_1(k) & B_2(k) & \cdots \\
B_2(k) & B_3(k) \\
\vdots & \ddots & \ddots \\
B_N(k)
\end{bmatrix},$$

(16)
where each $B_m(k)$ is a $U(2)$ matrix. Therefore, the map $f$ splits into $N$ maps

$$f_m : T^3 \rightarrow U(2), \quad m = 1, 2, \ldots, N.$$  \hspace{1cm} (17)

The next step is reducing $U(2)$ to $SU(2)$, which is a three-dimensional manifold. The motivation of this step will be clear later when we consider the degree of certain maps. To this end, we factorize $B_m(k) = \exp[i\theta_m(k)]u_m(k)$, where $u_m(k)$ is a $SU(2)$ matrix function of $k$. Because $\exp[i\theta_m(k)]u_m(k) = -\exp[i\theta_m(k)][-u_m(k)]$ and $-u_m(k)$ is also a $SU(2)$ matrix, there is ambiguity in this factorization. To avoid this ambiguity, we can choose a point $k_0$ in $T^3$, and choose one factorization $B_m(k_0) = \exp[i\theta_m(k_0)]u_m(k_0)$. The $U(1)$ factors of other $k$ points are determined by

$$\theta_m(k) = \theta_m(k_0) - \frac{i}{2} \int_{k_0}^{k} dk \nabla_k \ln(\det[B_m(k)]).$$  \hspace{1cm} (18)

It is easy to check that, with this equation, $u_m(k)$ will have unitary determinant. To make the integral in the above equation unambiguous, we require that $\oint_l dk \nabla_k \det[B_m(k)] = 0$ for arbitrary loop $l$ in $T^3$. For contractable loops, this is trivially satisfied. For non-contractable loops, considering the non-contractable loop AOB in figure 2 as an example, we have

$$\oint_{AOB} dk \nabla_k \ln(\det[B_m(k)]) = \int_{AO} dk \nabla_k \ln(\det[B_m(k)]) + \int_{OB} dk \nabla_k \ln(\det[B_m(k)]),$$

$$= 0$$  \hspace{1cm} (19)

which is a result of the relation $\det[B_m(-k)] = \det[B_m(k)]$. Therefore, we have a factorization of $U(2)$ into $SU(2)$ and $U(1)$. With this factorization, we also have $\oint_l dk \nabla_k \theta_m(k) = 0$ (for arbitrary loop $l$). Therefore, we can adiabatically deform the $U(1)$ factor to 1. Having got rid of the $U(1)$ factor, the maps $f_m : T^3 \rightarrow U(2)$ are deformed to $g_m : T^3 \rightarrow SU(2)$. This completes our discussion on matrix $B(k)$. With the aid of $B(k)$, we can give a geometrical interpretation of topological invariants of TR invariant topological insulators.
In order to prove the equivalence, we first show how to relate the topological invariant $P_3$ in (4) to a winding number. A similar formula appeared in [11] in a slightly different form but we would like to include the discussion here to make our discussion self-contained. We start from the integral topological invariants

$$P_3 = \frac{1}{16\pi^2} \int d^3k e^{ijk} \text{Tr}[[f_{ij}(k) - \frac{2}{3}i a_i(k) \cdot a_j(k)] \cdot a_k(k)],$$

which is valid independent of the TR symmetry. In a TR invariant system, with the aid of $B(k)$, we have

$$a_{i}^{\alpha \beta}(k) = -i (-k, \alpha | \partial_{k^\alpha} | - k, \beta)
= i \sum_{\alpha' \beta'} B_{\alpha' \beta'}(\Theta, k, \alpha' | \partial_k (B_{\alpha' \beta'}^* | \Theta, k, \beta'))
= i \sum_{\alpha' \beta'} B_{\alpha' \beta'}| \Theta, k, \alpha' | (\Theta, k, \beta') + i \sum_{\alpha' \beta'} B_{\alpha' \beta'} \partial_k B_{\alpha' \beta'}^*
= \sum_{\alpha' \beta'} B_{\alpha' \beta'}(a_{i}^{\alpha \beta}(k)) B_{\alpha' \beta'}^* + i \sum_{\alpha'} B_{\alpha' \beta'} \partial_k B_{\alpha' \beta'},$$

which can be simply written as

$$a_i(-k) = B(k) a_i^*(k) B^*(k) + i B(k) \partial_k B^*(k).$$

Therefore, the field strength satisfies the following relation

$$f_{ij}(-k) = \partial_{-k} a_j(-k) - \partial_{-k} a_i(-k) + i[a_i(-k), a_j(-k)]
= -B(k) f_{ij}^*(k) B^*(k).$$

These results imply that the non-Abelian Berry potential and curvature at $-k$ are simply related to those at $k$ by a non-Abelian gauge transformation $B(k)$. Therefore, we obtain that

$$P_3 = \frac{1}{16\pi^2} \int d^3k e^{ijk} \text{Tr}[[f_{ij}(-k) - \frac{2}{3}i a_i(-k) a_j(-k)] a_k(-k)]
= -\frac{1}{16\pi^2} \int d^3k e^{ijk} \text{Tr}[[f_{ij}(k) - \frac{2}{3}i a_i(k) a_j(k)] a_k(k)]^*
-\frac{i}{8\pi^2} \int d^3k e^{ijk} \text{Tr}[B^* a_j^* \partial_k B^*]
-\frac{1}{24\pi^2} \int d^3k e^{ijk} \text{Tr}[(B \partial_i B^*)(B \partial_j B^*)(B \partial_k B^*)]
= -P_3^* -\frac{1}{24\pi^2} \int d^3k e^{ijk} \text{Tr}[(B \partial_i B^*)(B \partial_j B^*)(B \partial_k B^*)]
= -P_3 -\frac{1}{24\pi^2} \int d^3k e^{ijk} \text{Tr}[(B \partial_i B^*)(B \partial_j B^*)(B \partial_k B^*)]$$

or

$$2P_3 = -\frac{1}{24\pi^2} \int d^3k e^{ijk} \text{Tr}[(B \partial_i B^*)(B \partial_j B^*)(B \partial_k B^*)].$$
Both the LHS and RHS of the above equation depend on gauge choices, but the parity of \(2P_3\) is gauge invariant

\[
2P_3(\text{mod } 2) = -\frac{1}{24\pi^2} \int d^3k e^{ijk} \text{Tr}[(B \partial_i B^\dagger)(B \partial_j B^\dagger)(B \partial_k B^\dagger)] \text{ (mod } 2),
\]

which is the important quantity for characterization of the topological insulator.

In our previous discussion, we have split \(B(k)\) into the direct sum of \(SU(2)\) matrices \((B_m, m = 1, 2, \ldots, N)\). It is readily obtained that

\[
2P_3(\text{mod } 2) = \sum_{m=1}^{N} v_m(\text{mod } 2),
\]

where

\[
v_m = -\frac{1}{24\pi^2} \int d^3k e^{ijk} \text{Tr}[(B_m \partial_i B_m^\dagger)(B_m \partial_j B_m^\dagger)(B_m \partial_k B_m^\dagger)].
\]

We note that \(v_m\) is just the winding number, or the integral form of degree of the map

\[
g_m : T^3 \rightarrow SU(2).
\]

The mod 2 degree of this map is given by

\[
\text{deg}_2(g_m) = v_m(\text{mod } 2).
\]

Therefore we have

\[
2P_3(\text{mod } 2) = \sum_{m=1}^{N} \text{deg}_2(g_m).
\]

This is the integral form of degree of the map. A natural question is whether we can find a discrete form, as discussed in the previous section. Let us denote the image of \(k\) under the map \(g_m\) as \(B_m(k)\), which is a \(SU(2)\) matrix. As has been noted, \(B_m(\Gamma_i)\) is antisymmetric at TRIM \(\Gamma_i\). There are only two antisymmetric matrices in \(SU(2)\), given by

\[
A_1 = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \quad A_2 = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}.
\]

It is easy to see that \(\text{Pf}[A_1] = 1\) and \(\text{Pf}[A_2] = -1\). In principle, we can pick any image point on the \(SU(2)\) to perform the counting for the degree of the map. However, because of the TR symmetry, the counting is particularly simple if we pick either \(A_2\) or \(A_1\). We now count the number of source points \(k\), modulo 2, which map onto \(A_2\). We first notice that if \(B_m(k) = A_2\), then \(B_m(-k) = -B_m^\dagger(k) = A_2\). Therefore, if \(k\) maps to \(A_2\), so does \(-k\). If \(k\) is not one of the TRIM, \(k\) and \(-k\) are distinct, and these two points do not contribute to \(\text{deg}_2(g_m)\), which counts the number of source points modulo 2. The only source points which may contribute to \(\text{deg}_2(g_m)\) are TRIM, where \(k\) and \(-k\) are equivalent. It is also important to note that the calculation of mod 2 degree of map is easier than that of the integer degree, which involves the \pm signs of the Jacobian of the map. Because \(-1 = 1(\text{mod } 2)\), we do not need to be concerned about the signs of the Jacobian when calculating degree of map mod 2.

Because we have reduced the map from \(U(2)\) to \(SU(2)\), \(\text{det}(B(\Gamma_i)) = 1\), we have \(\delta_i = \sqrt{\text{det}[B(\Gamma_i)]/\text{Pf}[B(\Gamma_i)]} = \text{Pf}[B(\Gamma_i)] = \prod_m \text{Pf}[B_m(\Gamma_i)]\). Suppose that there are \(n_m\) TRIMs...
which map onto $A_2$ under the map $g_m$ and $8 - n_m$ TRIMs which map onto $A_1$, by counting the number of points which map to $A_2$ mod 2, we have $\deg_2(g_m) = n_m (\mod 2)$, and therefore
\[( -1)^{2P_3} = (-1)^{\sum_{m=1}^{N} \deg_2(g_m)} = \prod_{m} (-1)^{n_m}. \tag{32} \]

On the other hand, the discrete invariant defined in [12] is given by
\[( -1)^{\nu_0} = \prod_{i} \text{Pf}[B(\Gamma_i)] = \prod_{i,m} \text{Pf}[B_m(\Gamma_i)] = \prod_{m} (-1)^{n_m}. \tag{33} \]

Therefore, we have proved the central result of this paper, namely the exact equivalence between the integral invariant of QHZ and the discrete invariant of FKM for the 3D topological insulator:
\[( -1)^{2P_3} = (-1)^{\nu_0}. \tag{34} \]

In the proof given above, we made the assumption that no accidental degeneracy except the Kramers degeneracy occurs, which simplified the discussion. The extension to the generic case is straightforward because $\pi_3(U(2N)) = \pi_3(U(2))$ holds for any integer $N \geq 1$. One can always deform the map $f$ to one of the $U(2)$ subgroups of $U(2N)$, so that the proof discussed above applies.

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Appendix. Discussion on the global basis of wavefunctions

In this appendix we shall show that the global basis of wavefunctions exists on $T^3$ in the presence of TR symmetry. Because the global definition of $B(k)$ and the discrete invariant $\nu_0$ depends on the existence of such a global basis, this point is important to our argument.

We divide the $2N$ filled bands into $N$ TR pairs. Within each pair, the Hilbert space is 2D at each momentum $k$. Therefore, the Hilbert space is naturally a $U(2)$ fibre bundle on $T^3$. Generically it is not evident that this bundle is trivial. The key to the existence of the global basis is the TR symmetry.

The ‘surface’ of the cubic in figure 2 consists of three $T^2$ (2D tori). We consider the restriction of the $U(2)$ bundle to one of these tori. The bundle on $T^2$ is trivial because the first Chern number $C_1 = 0$, which is a consequence of TR symmetry. Therefore, a global basis exists on the surface of the cubic. Such a basis can be extrapolated to the interior of the cubic since the the interior region is topologically trivial. We consider the transition function between the surface and the interior region on their overlapping region, which is topologically equivalent to $S^2$(two-dimensional sphere). Because the second homotopy group $\pi_2(U(2))$ is trivial, mappings from $S^2$ to $U(2)$ (the structure group of the fibre bundle) are all trivial. Thus the bundle is trivial on $T^3$. Therefore, the global basis does exist.

For comparison, we note that in the case of integer QH states, the global basis does not exist on the Brillouin zone $T^2$, because the relevant fibre bundle on $T^2$ is nontrivial. From this example we also see that TR symmetry is necessary for our argument.

New Journal of Physics 12 (2010) 065007 (http://www.njp.org/)
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New Journal of Physics 12 (2010) 065007 (http://www.njp.org/)