An equivalent expression of $Z_2$ Topological Invariant for band insulators using Non-Abelian Berry’s connection

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We introduce a new expression for the $Z_2$ topological invariant of band insulators using non-Abelian Berry’s connection. Our expression can identify the topological nature of a general band insulator without any of the gauge fixing problems that plague the concrete implementation of previous invariants. The new expression can be derived from the "partner switching" of the Wannier function center during time reversal pumping and is thus equivalent to the $Z_2$ topological invariant proposed by Kane and Mele.

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I. INTRODUCTION

Topological insulators play a very important role in the classification of band insulators. The studies on integer quantum Hall effect (IQHE) show that 2D band insulators without time reversal symmetry can be classified by the Chern number - an integer describing the topological structure of a set of fully occupied Bloch bands without Kramers degeneracy. Systems with non-zero Chern number exhibit IQHE. A similar idea can be also applied to band insulators with time reversal symmetry. Recently a $Z_2$ topological invariant has been proposed by Kane and Mele to characterize the time reversal invariant band insulators in 2D. According to this new topological invariant, all the 2D band insulators with time-reversal invariance can be divided into two classes. The normal insulators with even $Z_2$ number and topological insulators with odd $Z_2$ number exhibit IQHE. The 2D topological insulators will exhibit a quantum spin Hall effect (QSHE), which is characterized by the presence of helical edge states. Interestingly the $Z_2$ topological invariant can also be generalized to the 3D band insulators with time reversal symmetry. In this case, there are four independent $Z_2$ topological numbers: one strong topological index and three weak topological indices. The 3D time reversal invariant band insulators can be classified as normal insulators, weak topological insulators (WTI) and strong topological insulators (STI) according to the values of these four $Z_2$ topological indices. Among them, the STI attracts much attention due to its unique Dirac type surface states and robustness against disorder. The helical spin structure of the Dirac type surface states has been experimentally implied by the standing wave structure in STM images around an impurity scattering center and measured directly by spin resolved angle resolved photo emission spectra (ARPES). The Dirac type 2D electron gas living on the surface of STI or at the interface between STI and normal insulators provides a new playground for spintronics and quantum computing.

Since the $Z_2$ invariant characterizes whether a system is topologically trivial or nontrivial, its computation is essential to the field of topological insulators. For band insulators with extra spacial inversion symmetry, the $Z_2$ topological numbers can be easily computed as the product of half of the parity (Kramers pairs have identical parities) numbers for all the occupied states at the high symmetry points. The situation becomes complicated in the general case where spacial inversion symmetry is absent. At the present, numerically there are three different ways to judge if a band insulator without inversion symmetry is a TI or not. i) Compute the $Z_2$ numbers using the integration of both Berry’s connection and curvature over half of the Brillouin Zone (BZ). In order to do so, one has to set up a mesh in the k-space and calculate the corresponding quantities on the lattice version of the problem. Since the calculation involves the Berry’s connection, one has to numerically fix the gauge on the half BZ, which is not easy for the realistic wave functions obtained by first principle calculation. ii) Start from an artificial system with spacial inversion symmetry, and then smoothly "deform" the Hamiltonian towards the realistic one without inversion symmetry. If the energy gap never closes at any points in the BZ during the "deformation" process, the realistic system must share the same topological nature with the initial reference system whose $Z_2$ number can be easily counted by the inversion eigenvalue formula. Unfortunately making sure that the energy gap remains open on the whole BZ is very difficult numerically, especially in 3D. iii) Directly calculate the surface states. For most of the TI materials, the first principle calculation for the surface states is numerically heavy. Therefore it is valuable to develop a mathematically equivalent way to calculate the $Z_2$ numbers of a band insulator, which satisfies the following conditions: first it should use only the periodic bulk system; second, it should not require any gauge fixing condition - thereby greatly simplifying the calculation; third, it should be easily applied to general systems lacking spacial inversion symmetry.
In the present paper we propose a new equivalent expression for the $Z_2$ topological invariant using the U(2N) non-Abelian Berry connection. Based on this new expression, we further propose a new numerical method to calculate the $Z_2$ topological number for general band insulators, without choosing a gauge fixing condition. The main idea of the method is to calculate the evolution of the Wannier function center directly during a "time reversal pumping" process, which is a $Z_2$ analog to the charge polarization. We derive that the center of the Wannier function for the effective 1D system can be expressed as the U(1) phase of eigenvalues of a matrix obtained as the product of the U(2N) Berry connection along the "Wilson loop". The $Z_2$ topological numbers can be expressed as the number of times mod 2 of the partner switching of these phases during a complete period of the "time reversal pumping" process. Using this new method, we have recalculated the $Z_2$ topological numbers for several TI systems, including strained HgTe, Bi, Sb and Bi$_2$Se$_3$, and found the "partner switching" patterns, which differentiate between topologically trivial and nontrivial behavior. The rest of paper will be organized as follows: in section II we derive the new mathematical form of the $Z_2$ numbers through the "Wilson loop"; we apply the new method to various TI systems in section III; we prove the equivalence of the new methods and the $Z_2$ number propose by Fu and Kane in the appendices.

II. THE FORMALISM

The Bloch wave functions describing the band structure of a translationally invariant system can be expressed in terms of a complete set of local basis labeled by the unit cell $i$ and some other quantum number $\alpha$ as:

$$|\psi_{nk}(r)\rangle = \frac{1}{\sqrt{N}} \sum_{\alpha} u_{\alpha nk}(k) e^{i k \cdot R_i} |\phi_\alpha(r - R_i)\rangle$$  

(1)

We will first focus on the 2D system. The topological nature of a 3D insulator can be determined by looking at these effective 2D systems with fixed $k_i = 0$ and $k_i = \pi$ ($i = x, y, z$).

Following Fu and Kane, for a 2D insulator we can further reduce the dimension by fixing $k_y$ and study the "time reversal" pumping process with the adiabatic change of $k_y$. The main idea of our new formalism is to directly look at the evolution of Wannier centers for these effective 1D systems in the subspace which contains only occupied states. Fixing $k_y$, we can define the position operator for the effective 1D system as

$$\hat{X} = \sum_{ia} e^{i \delta k_x R_i} |\phi_\alpha(r - R_i)\rangle |\phi_\alpha(r - R_i)\rangle$$  

(2)

where $\delta k_x = \frac{2\pi}{N_x a_x}$, $N_x$ is the number of real-space unit cells along the $x$ direction, $a_x$ is the lattice constant, $\alpha$ is the orbital and spin index and $R_i$ labels the unit cell. The operator $\hat{X}$ is a unitary operator with all the eigenvalues being $e^{i \delta k_x R_i}$, whose phase represents the position. The eigenvalue of the position operator can be viewed as the center of maximum localized Wannier function (MLWF) formed by the bands included in the operator $\hat{X}$. Because the local basis set $\alpha$ is assumed to be complete, such MLWFs are always well defined. As pointed out by Fu and Kane, the $Z_2$ topological invariant can be determined by looking at the evolution of the Wannier function center for the effective 1D system with fixed $k_y$ in the subspace spanned by the occupied bands only. Therefore we should consider the eigenvalue of the projected position operator defined as

$$\hat{X}_P = \hat{P} \hat{X} \hat{P}$$

$$= \sum_{nm\in\alpha} \sum_{k_j, k_j'} e^{i \delta k_x R_i} |\psi_{nk_x k_y}\rangle \langle \psi_{nk_x k_y}|$$

$$\times |\phi_\alpha(r - R_i)\rangle |\phi_\alpha(r - R_i)\rangle$$

$$= \sum_{nm\in\alpha} \sum_{k_j, k_j'} e^{i (k_x + \delta k_x - k_y')} R_i |\psi_{nk_x k_y}\rangle \langle \psi_{nk_x k_y}|$$

$$\times \sum_{\alpha} u_{\alpha nk_x}(k_j) u_{\alpha nk_y}(k_j')$$

$$= \sum_{k_x, k_y'} \delta(k_x + \delta k_x - k_y') \sum_{nm\in\alpha} |\psi_{nk_x k_y}\rangle \langle \psi_{nk_x k_y}|$$

$$\times \sum_{\alpha} u_{\alpha nk_x}(k_j) u_{\alpha nk_y}(k_j')$$

(3)

where $\alpha$ means the occupied bands. The above operator can be written in a more suggestive matrix form

$$\hat{X}_P(k_y) =$$

$$\begin{bmatrix}
0 & F_{0,1} & 0 & 0 & 0 & 0 \\
0 & 0 & F_{1,2} & 0 & 0 & 0 \\
0 & 0 & 0 & F_{2,3} & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & \cdots \\
0 & 0 & 0 & 0 & 0 & F_{N_x - 2, N_x - 1} \\
F_{N_x - 1, 0} & 0 & 0 & 0 & 0 & 0
\end{bmatrix}$$  

(4)

where $F_{n,m}^{i,i+1}(k_y) = \sum_{\alpha} u_{\alpha nk_x, k_y} u_{\alpha nk_{x,i+1}, k_y} u_{\alpha nk_{x,i+1}, k_{y+1}}$ are the $2M \times 2M$ matrices spanned in $2M$ occupied states and $k_{x,i} = \frac{2\pi i}{N_x a_x}$ are the discrete $k$ points taken along the $x$-axis.

The eigen problem of $\hat{X}_P(k_y)$ can be solved by the transfer matrix method. We can define a product of $F_{i,i+1}$ as

$$D(k_y) = F_{0,1} F_{1,2} F_{2,3} \cdots F_{N_x - 2, N_x - 1} F_{N_x - 1, 0}$$  

(5)

$D(k_y)$ is a $2M \times 2M$ matrix, which has $2M$ eigenvalues:

$$\lambda_m^D = |\lambda_m^D| e^{i \theta_m^D} \quad m = 1, 2, \cdots, 2M$$
where \( \theta^D_m \) is the phase of the eigenvalues:

\[
\theta^D_m = \text{Im}(\log |\lambda^D_m|)
\]

(6)

We can easily prove that the eigenvalue of projected position operator \( X_P \) can be simply related to the eigenvalue of the above D-matrix by

\[
|\lambda^D_{m,n}| = \sqrt{\lambda^D_m} = \sqrt{|\lambda^D_m|e^{i(\theta^D_m + 2\pi n)/N_x}}
\]

(7)

where \( n = 1, 2, \ldots, N_x \). We can further prove that the D-matrix is unitary and all the \( |\lambda^D_m| \) equals one.

The evolution of the Wannier function center for the effective 1D system with \( k_y \) can be easily obtained by looking at the phase factor \( \theta^D_m \). At \( k_y = 0 \), the eigenvalues of the D-matrix appear in degenerate pairs due to time reversal symmetry, which results in pairs of Wannier centers sitting at \( k_y = 0 \). When \( k_y \) moves away from the origin, the Wannier center pairs split and recombine at \( k_y = \pi \), as shown in Fig.1. Because \( \theta^D_m \) is a phase factor, when two \( \theta^D_m \)'s meet together, they may differ by integer times of \( 2\pi \). Therefore the evolution of each Wannier center pair will enclose the whole cylinder an integer times, which can be viewed as the winding number of the Wannier center pair. The \( Z_2 \) topological number is related to the summation of the winding numbers for all the pairs. If it is odd, then the \( Z_2 \) topological number is odd. It seems that the total winding number of the Wannier center pairs should generate an integer class \( Z \) instead of \( Z_2 \). To clarify this point, let’s look at the evolution of a Wannier center pair with winding number \( 4\pi \).

In that particular case, as shown in Fig.1(C), the pair of Wannier centers must have an extra "accidental" degeneracy between \( k_y = 0 \) and \( \pi \), which is not protected by any symmetry and can be removed by "deforming" the Hamiltonian slightly to make the crossing of the levels become an anti-crossing as shown in Fig.1(C). The "deformation" process will thus change the total winding number by \( 4\pi \) and make it 0. Therefore only the total winding number mod 2 is a topological invariant.

The eq. (6) can be viewed as the discrete expression of the Wilson loop for the U(2M) non-Abelian Berry’s connection. It is obviously invariant under the U(2M) gauge transformation and thus can be calculated directly from the wave functions obtained by first principle method without choosing any gauge fixing condition, which is the biggest advantage of the present form of the \( Z_2 \) invariance. The equivalence to the \( Z_2 \) number proposed by Kane and Mele will be proved rigorously in the appendix.

### III. NUMERICAL RESULTS

In the present section, we will implement the method and explicitly compute the \( Z_2 \) invariant for a series of systems. For each particular system, we calculate the evolution of the \( \theta^D \) defined in equation (6) as the function of \( k_y \) from zero to \( \pi \). The winding number of the Wannier center pairs defined in the above section can be checked in an equivalent way which is much simpler in practice. We first draw an arbitrary reference line parallel to the \( k_y \) axis, then compute the \( Z_2 \) number by counting how many times the evolution lines of the Wannier centers crosses the reference line.

#### A. BHZ model

Bernevig Hughes and Zhang (BHZ) showed that for an appropriate range of well thickness, the HgTe/CdTe quantum well exhibits an inverted sub-band structure. In this inverted regime, the system exhibits a 2D quantum spin Hall effect\(^{13}\). BHZ introduce a simple four band tight binding model to describe this effect:

\[
H_{eff}(k_x, k_y) = \begin{bmatrix}
H(k) & 0 \\
0 & H^*(-k)
\end{bmatrix}
\]

(8)
where \( H(k) = \varepsilon(k) + d_1(k)\sigma_i, \) \( d_1 + id_2 = A[\sin k_x + i\sin k_y], d_3 = -2B[2 - \frac{i\sin k_x}{\cos k_x - \cos k_y}],\) \( \varepsilon(k) = C - 2D[2 - \cos k_x - \cos k_y]. \) Real HgTe does not have inversion symmetry but the BHZ toy model does. To describe the inversion symmetry breaking effect we add a new term \( H': \)

\[
H' = \begin{bmatrix}
0 & 0 & 0 & \Delta \\
0 & 0 & -\Delta & 0 \\
0 & -\Delta & 0 & 0 \\
\Delta & 0 & 0 & 0
\end{bmatrix}
\]

(9)

We apply the new method to calculate the shift of the Wannier function center based on the above model Hamiltonian and show the results in Fig. 2.

![Figure 2: Wannier centers for the BHZ model. (A) For the QSH phase (A=-13.68, B=-16.9, C=-0.0263, D=-0.514, M=-2.058, \( \Delta = 1.20 \)), The Wannier center cross the reference line (red dashed line) once (odd times); (B) For the Normal insulating phase (A=-14.48, B=-18.0, C=-0.018, D=-0.594, M=-2.766, \( \Delta = 1.20 \)), The Wannier center cross the reference line (red dashed line) zero (even) times.](image)

To show these results more clearly, we glue \( \theta = -\pi \) line and \( \theta = \pi \) line together. Then the Wannier centers live on a cylinder surface. The corresponding results for the QSH phase are showed in Fig 2(A). When moving from \( k_y = 0 \) to \( \pi \) we see that the two evolution lines of Wannier centers enclose the cylinder once and equivalently these evolution lines cross the reference line (the red dashed line) once (odd times). By contrast, for the normal insulator phase, as shown in Fig 2(B), the two evolution lines of Wannier centers never cross the reference line. Therefore in the BHZ toy model for TI, the \( Z_2 \) number calculated by our new method is consistent with the previous conclusion. Next we will apply the method to more realistic models of insulating materials.

### B. CdTe and HgTe

The CdTe and HgTe materials have a similar zinc-blende structure without bulk inversion symmetry. CdTe has an normal electronic structure, where the conduction bands (\( \Gamma_6 \)) have the s-like character and the valance bands have the p-like character (\( \Gamma_8 \)) throughout the whole Brillouin Zone. In HgTe, the band structure is inverted in a small area near the \( \Gamma \) point, where the s-like \( \Gamma_6 \) band sinks below the p-like \( \Gamma_8 \) band. The band inversion at the \( \Gamma \) point changes the topological nature of the band structure and makes the HgTe to be the topological insulator if a true energy gap is opened by the lattice distortion. As pointed out in ref.\(^7\), the uniaxial strain is applied along the \([001]\) direction for HgTe by choosing the \( c/a \) ratio to be 0.98 and the energy gap is about 0.05eV at the \( \Gamma \) point. We then apply a tight-binding model\(^4\) to calculate the pattern of the Wannier center evolution \( \theta \) defined in Eq 6 and show the results in Fig 2. It is very clear that in the HgTe system, for \( k_z = 0 \) the evolution line crosses the reference line (red dashed line) once (as shown in Fig 2A), while for \( k_z = \pi \) it never crosses (as shown in Fig 2B). The above results indicate that in the case of HgTe the effective 2D systems for fixed \( k_z = 0 \) and \( \pi \) are effectively 2D topological insulator and normal insulator respectively, which determines HgTe to be a strong 3D topological insulator. A similar analysis can be also applied to CdTe and the results are shown in Fig 2(C) and (D). They clearly indicate that CdTe is a normal insulator.

### C. Bi\(_2\)Se\(_3\) system

Recently, the tetradymite semiconductors Bi\(_2\)Te\(_3\), Bi\(_2\)Se\(_3\), and Sb\(_2\)Te\(_3\) have been theoretically predicted and experimentally observed to be topological insulators (TI) with a bulk band gap as large as 0.3eV in Bi\(_2\)Se\(_3\).\(^{20,21,23,25,26,39}\) The Bi\(_2\)Se\(_3\) surface state has been found by both ARPES\(^{21,24}\) and STM\(^{25}\), consistent with the theoretical results\(^\text{20}\). Since the Bi\(_2\)Se\(_3\) family has inversion symmetry, the \( Z_2 \) topological number can be easily calculated by the product of half the parities at each high symmetry points in the Brillouin Zone.\(^\text{36}\) Below we apply our new method to calculate the topological property of this system, using the tight binding model based on the Wannier functions obtained in reference\(^\text{20}\). We first perform the calculation for the Bi\(_2\)Se\(_3\) without spin-orbit coupling: the results are shown in Fig 3(A,B). It is clear that the evolution lines never cross the reference line for both \( k_z = 0 \) and \( \pi \), indicating that the system is topologically trivial without spin-orbital coupling. When the realistic spin orbital coupling is turned on, as shown in Fig 3(C,D), the evolution lines cross the reference line once only in the case of \( k_z = 0 \) but not for \( k_z = \pi \) indicating the Bi\(_2\)Se\(_3\) bulk material is a 3D strong topological insulator.
Figure 3: The evolution lines of Wannier centers for HgTe (A, B) and CdTe (C, D). For HgTe system, The Wannier center cross the reference line odd times in the $k_z = 0$ plane and even times in the $k_z = \pi$ plane, indicating HgTe is a strong topological insulator. For CdTe, the Wannier centers cross the reference line zero times for both $k_z = 0$ and $\pi$ planes, indicating CdTe is a normal insulator.

Figure 4: The evolution lines of Wannier centers for Bi$_2$Se$_3$ system without (A, B) and with SOC (C, D). If we turn off SOC the system is a normal insulator and the Wannier centers never cross the reference line for both $k_z = 0$ and $\pi$ planes as shown in (A) and (B), indicating it is a normal insulator. When the SOC is turned on the system is in a strong topological phase, the Wannier centers cross the reference line odd times in $k_z = 0$ and even times in $k_z = \pi$ plane, as shown in (C) and (D), indicating the system is topologically non-trivial.
D. \( \text{Bi}_2\text{Te}_3 \) slab system

As calculated by Liu et al.\(^46\), upon reducing the thickness of \( \text{Bi}_2\text{Te}_3 \) and \( \text{Bi}_2\text{Se}_3 \) films, the topological nature of the system alternates between topologically trivial and non-trivial behavior as a function of the layer thickness. Liu et al.\(^46\) point out that the 1QL \( \text{Bi}_2\text{Te}_3 \) slab is a trivial insulator and 2QL \( \text{Bi}_2\text{Te}_3 \) slab is a 2D topological insulator.\(^46\) We apply our method to these systems. The evolution patterns for the 1QL and 2QL \( \text{Bi}_2\text{Te}_3 \) slabs are obtained using the tight binding Hamiltonian developed in references\(^46,47\) and the results are summarized in Fig. 5. In the 1QL slab system (Fig. 5(A)), the evolution pattern appears in a trivial manner while that of the 2QL slab system is non-trivial (Fig. 5(B)). This is consistent with the conclusion based on the parity counting\(^46\).

![Figure 5: The evolution lines of Wannier centers for 1QL and 2QL \( \text{Bi}_2\text{Te}_3 \) slab. (A) The 1QL \( \text{Bi}_2\text{Te}_3 \) slab is in normal insulator phase. (B) The 2QL \( \text{Bi}_2\text{Te}_3 \) slab is in topological insulator phase.](image)

E. \( \text{Bi} \) and \( \text{Sb} \) system

Murakami pointed out that the \( \mathbb{Z}_2 \) topological number is odd in the 2D bilayer bismuth system.\(^48\) We apply our method to this system using the tight-binding model developed in reference\(^49\), which faithfully reproduces the bulk bismuth band structure. As shown in Fig. 6(A), the band structure of bilayer bismuth is topologically nontrivial, which is quite consistent with the previous conclusion.\(^48\) After that we apply the same method to calculate single-bilayer Sb, which has the similar lattice structure as bismuth, but with relatively weak SOC. As plotted in Fig. 6(B), the evolution pattern of bilayer Sb shows clearly that it is in the normal insulator phase, which is also consistent with the parity counting.

![Figure 6: The evolution lines of Wannier centers for 2D single-bilayer Bi (A) and Sb (B) system, indicating the single-bilayer Bi is topologically nontrivial but Sb is topologically trivial.](image)

F. Graphene system

In 2005 Kane and Mele pointed out\(^4\) that there are two different phases in graphene, depending on the spin-orbital coupling \( \lambda_R \) and the staggered sublattice potential parameter \( \lambda_v \). The system is in a quantum spin Hall (QSH) phase when \( \lambda_v = 0 \) and normal insulator phase when \( \lambda_v = 0.4t \), where \( t \) is the hopping parameter. In the present study, we use the same parameters as Kane and Mele to calculate the corresponding Wannier center evolution pattern. The results are shown in Fig. 7. It can be easily found that there is one partner switching in Fig. 7(A) but not in Fig. 7(B) indicating the former is topologically non trivial and the latter is trivial.
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Wannier functions is not necessary, while only the Wannier expressions we calculated the evolution of the Wannier functions center for graphene phase \( \lambda \), and (B) the normal insulating \( \theta(2\pi) \). In both cases \( \lambda_{SO} = 0.06t \) and \( \lambda_R = 0.05t \).

In conclusion, we have proposed a new equivalent expression for the \( Z_2 \) topological invariance using the \( U(2N) \) non-Abelian Berry connection. Based on this new expression we calculated the evolution of the Wannier function center for several topological and normal insulating systems with or without inversion symmetry. We showed that for the nontrivial topological insulators, the Wannier function center have partner switching patterns, topologically different from the normal (trivial) insulating systems. Additionally, we gave a proof that the new method is equivalent to the \( Z_2 \) number proposed by Fu and Kane.

**Note** During the preparation of this manuscript, we noticed the paper by Soluyanov and Vanderbilt\(^{25} \), where the construction of Wannier functions for \( Z_2 \) topological insulators are discussed from a different view of point. We addressed in this paper that the real construction of Wannier functions is not necessary, while only the "Wannier representation" and corresponding Berry connection evaluated along the "Wilson loop" are essential keys in order to identify the topological nature.

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### Appendix A: Proof of gauge invariance of the \( D(k_y) \) operator and its equivalence to the \( U(2) \) wilson loop

We first give the proof of gauge invariance of the \( D(k_y) \) operator and its equivalence to the \( U(2) \) Wilson loop. The \( D(k_y) \) operator is, at each \( k_y \), the product:

\[
D(k_y) = F_{0,1}F_{1,2}F_{2,3}F_{N_x-2,N_x-1}F_{N_x-1,0}
\]

where

\[F_{i,i+1}^{mn} = \langle m, k_{x,i}, k_y| n, k_{x,i+1}, k_y \rangle \]

\( k_{x,i} = i\Delta k \), \( \Delta k = \frac{2\pi}{N_x} \), and let \( k_{x,N_x} = 0 \) to make \( k_x \) go back to the initial point. \( m, n \) are running through from 1 to the number of occupied bands, \( |n, \vec{k}| \) is the \( n \)’th wavevector of energy \( E_n \) of the insulating Hamiltonian:

\[
H(\vec{k})|n, \vec{k}\rangle = E_n|n, \vec{k}\rangle
\]

For a fixed \( k_y \), the \( k_x = [-\pi, \pi] \) interval is broken up in \( N_x \) parts. This corresponds to periodic boundary conditions in the \( x \) direction and \( N_x \) sites. \( D(k_y) \) operator is then:

\[
D_{mn}(k_y) = [F_{0,1}F_{1,2}F_{2,3}F_{N_x-2,N_x-1}F_{N_x-1,0}]_{mn}
\]

\[
= \langle m, k_0| n_1, k_1 \rangle \langle n_1, k_1| n_2, k_2 \rangle \cdots \langle n_{N_x-2}, k_{N_x-2}| n_{N_x-1}, k_{N_x-1} \rangle \langle n_{N_x-1}, k_{N_x-1}| n, k_0 \rangle
\]

where double index of \( n_i \) implies summation. As the \( k_y \) index is self-understood, we will suppress it at times and re-introduce it when necessary.

Under a unitary transformation \( |n, \vec{k}\rangle \rightarrow \sum_{m} M_{mn}(\vec{k}) |m, \vec{k}\rangle \)

and hence \( D(k_y) \) matrix goes into

\[
D_{mn}(k_y) \rightarrow M_{mn}(k_0) |m', k_0| n', k_1 \rangle \cdot M_{n', n_1}(k_1) \cdots M_{n, n_1}(k_1) |k_{N_x-2}, n, k_{N_x-2} \rangle \cdot |n', k_{N_x-1}, k_{N_x-1} \rangle \cdot M_{n', n_1}(k_1) \cdots \langle n_{N_x-1}, k_{N_x-1}| n', k_0 \rangle M_{n, n'}(k_0)
\]

or

\[
M_{m', m}(k_0) |m', k_0| n, k_1 \rangle \cdot M_{n, n_1}(k_1) \cdots M_{n, n_1}(k_1) \cdot |k_{N_x-2}, n, k_{N_x-2} \rangle \cdot |n_{N_x-1}, k_{N_x-1} \rangle \cdot M_{n', n_1}(k_1) \cdots \langle n_{N_x-1}, k_{N_x-1}| n', k_0 \rangle M_{n, n'}(k_0)
\]
where $A$ and $U$ with $\beta$ invariance we can relate the bands at $k$ goes across the BZ in $k$ or equivalently:

$$F_{-k_x-k_y} = B(k_2)F^T_{k_1,k_2}B^T(k_1)$$ (B4)

We now focus on the $k_y = 0$ or $k_y = \pi$ paths (say $k_y = 0$), each of which has $k_x$ going from $-\pi$ to $\pi$, so that $k_y = -k_y$, and compute the finite difference:

$$D(k_y = 0) = \prod_{i=0}^{N_y-1} F_{i,i+1}$$

$$= F_{-\frac{\Delta k}{2}} - (\frac{\Delta k}{2} - 1) \Delta k \cdots F_{-3\Delta k,-2\Delta k}F_{-2\Delta k,-\Delta k} \times F_{-\Delta k,0} F_{0,\Delta k} F_{\Delta k,2\Delta k} \cdots F_{(\frac{\Delta k}{2} - 1)\Delta k, \frac{\Delta k}{2} \Delta k}$$ (B5)

where again we are at $k_y = 0$ for all the $F$'s in the above, and the $k$ in the above expresses the $k_x$ coordinate. By the above $F_{-k_x-k_y} = B(k_2)F^T_{k_1,k_2}B^T(k_1)$, we have:

$$F_{-2\Delta k,-\Delta k} = B(2\Delta k)F^T_{\Delta k,2\Delta k}B^T(\Delta k), \cdots$$ (B6)

Hence the Wilson loop above becomes:

$$D = B(\frac{N_y}{2} \Delta k)F^T_{(\frac{\Delta k}{2} - 1)\Delta k, \frac{\Delta k}{2} \Delta k} \cdots F_{(\frac{\Delta k}{2} - 1)\Delta k, \frac{\Delta k}{2} \Delta k}$$

$$B_{(\frac{\Delta k}{2} - 2)\Delta k, (\frac{\Delta k}{2} - 1)\Delta k} F^T_{(\Delta k)\frac{\Delta k}{2} \Delta k} \cdots$$

$$F^T_{(\frac{\Delta k}{2} - 2)\Delta k, (\frac{\Delta k}{2} - 1)\Delta k} F^T_{(\frac{\Delta k}{2} - 1)\Delta k, \frac{\Delta k}{2} \Delta k}$$ (B7)

where we have used the fact that $B^T(k)B(k) = I$ (unitary matrix). We hence see that all the intermediate B matrices vanish with the exception of the ones at the inversion symmetric points $0, \frac{\Delta k}{2} \Delta k$. This is obviously true for any time-reversal invariant contour. Moreover, it is suggestive that the two left-over matrices $B^T(0), B(\frac{\Delta k}{2} \Delta k)$ be brought together, so we must commute $B^T(0)$ all across the matrix chain.

The matrix $B(0)$ (and $B(\pi)$) has the property that it is unitary and antisymmetric, per $B(k) = B^T(-k)$ in eq. We then have:

$$B(0) = e^{i\theta} \sigma_2$$ (B8)

The matrix $F_{k_1,k_2}$, for $k_2 - k_1 \ll \pi$, as shown in eq. has the following form:

$$F^T_{k_1,k_2} = \delta_{mn} + A_{k_1,k_2}(k_2 - k_1)$$ (B9)

$$D(k_y) \rightarrow M^T(k_0)D(k_y)M(k_0)$$

which means that the eigenvalues of $D(k_y)$ (or its trace and determinant) remain unchanged under a $U$ (occupied) gauge transformation.

For infinitesimal $\Delta k \ll 2\pi$, we have:

$$F^m_{n,i+1} = \langle m,k_{x,i},k_y|n,k_{x,i+1},k_y \rangle$$

$$= \delta_{mn} + \langle m,k_{x,i},k_y|((n,k_{x,i+1},k_y) - |n,k_{x,i},k_y) \rangle$$

$$= \delta_{mn} + A_{mn} \Delta k$$

$$\approx e^{i\Delta A_{mn} \Delta k}$$ (A6)

where $A_{mn} = \frac{\langle m,k_{x,i},k_y|n,k_{x,i},k_y - |n,k_{x,i},k_y \rangle}{\Delta k}$ is the non-abelian $U$ (occupied) gauge field. Hence we have that $D(k_y)$ is:

$$D(k_y) = \prod_{i=0}^{N_y-1} F_{i,i+1} = \prod_{i=0}^{N_y-1} e^{iA_{i,i+1} \Delta k}$$

This is just the $U$ (occupied) (not $SU$ (occupied)) Wilson loop, where the contour $C_{k_y}$ is a contour at fixed $k_y$ which goes across the BZ in $k_x$, i.e. goes from $k_x = -\pi$ to $k_x = \pi$, through $k_x = 0$.

Appendix B: Wilson loop and pfaffian topological invariant

In this section, we will prove that the $U(2)$ Wilson loop is related to the topological invariant of time-reversal topological insulators. In a system with time-reversal invariant we can relate the bands at $k$ and $-k$ through a unitary matrix $B$,

$$|n,-k) = B^*_m(k)\tilde{T}|m,k)$$ (B1)

with $B(k)$ unitary and has the property:

$$B(-k) = -B^T(k)$$ (B2)

We have the following relation between $F_{k_1,k_2}$ matrices:

$$F^m_{-k_x,-k_y} = \langle m,-k_x|n,-k_y \rangle$$

$$= \langle m',k_2|\tilde{T}B_{mn}B^*_{mn}\tilde{T}|n',k_1 \rangle$$

$$= B_{mn}B^*_{mn}\tilde{T}F^m_{n,m'}$$

$$= B_{mn}(F^T_{k_1,k_2})\tilde{T}F^m_{n,m'}B^T_{m'n}$$ (B3)

or equivalently:

$$F^m_{k_1,k_2} = \delta_{mn} + A_{k_1,k_2}(k_2 - k_1)$$ (B9)
where \( k_2 - k_1 = \Delta k \). We decompose the \( U(2) \) gauge field into its abelian and non-abelian part:

\[
A^{mn}_{k_1,k_2} = A^{U(1)}_{k_1,k_2} \delta_{mn} + A^{SU(2),i}_{k_1,k_2}(\sigma^i)_{mn}
\]

where \( i = 1, 2, 3 \) and double index implies summation. \( A^{U(1)}_{k_1,k_2}, A^{SU(2),i}_{k_1,k_2} \) are numbers. We have:

\[
(F^T)_{k_1,k_2}^{mn} = (F_{k_1,k_2})^{mn} = \delta_{mn} + (A^{U(1)}_{k_1,k_2})^{\delta_{mn}} + A^{SU(2),i}_{k_1,k_2}(\sigma^i)^T_{mn}(k_2 - k_1) \quad \text{(B11)}
\]

We have that:

\[
(F^T)_{k_1,k_2} B^\dagger(0) = B^\dagger(0) (I + A^{U(1)}_{k_1,k_2}(k_2 - k_1)I) + A^{SU(2),i}_{k_1,k_2}(\sigma^i)^T(k_2 - k_1) B^\dagger(0) \quad \text{(B12)}
\]

we have commuted the first two terms easily as they are proportional to the identity, but the last term required a bit more work:

\[
\sigma^T \sigma_y = -\sigma_y \sigma_x
\]

\[
\sigma^T \sigma_y = -\sigma_y \sigma_y
\]

\[
\sigma^T \sigma_y = -\sigma_y \sigma_z
\]

and hence:

\[
A^{SU(2),i}_{k_1,k_2}(\sigma^i)^T B^\dagger(0) = e^{-i\theta} A^{SU(2),i}_{k_1,k_2}(\sigma^i)^T \sigma_2
\]

\[
= -e^{-i\theta} A^{SU(2),i}_{k_1,k_2}(\sigma^i)^T \sigma^i = -B^\dagger(0) A^{SU(2),i}_{k_1,k_2}(\sigma^i)^T \quad \text{(B14)}
\]

Hence:

\[
(F^T)_{k_1,k_2} B^\dagger(0) = B^\dagger(0) (I + A^{U(1)}_{k_1,k_2}(k_2 - k_1)I - A^{SU(2),i}_{k_1,k_2}(\sigma^i)^T(k_2 - k_1)]
\]

\[
= B^\dagger(0) (I + A^{U(1)}_{k_1,k_2}(k_2 - k_1)I - A^{SU(2),i}_{k_1,k_2}(\sigma^i)^T(k_2 - k_1)] + 2 A^{U(1)}_{k_1,k_2}(k_2 - k_1)
\]

We also have

\[
I - (A^{U(1)}_{k_1,k_2} I + A^{SU(2),i}_{k_1,k_2}(\sigma^i)(k_2 - k_1) + 2 A^{U(1)}_{k_1,k_2}(k_2 - k_1))
\]

\[
= (A_{k_1,k_2} I + 2 A^{U(1)}_{k_1,k_2}(k_2 - k_1))I
\]

\[
\approx (I + A^{U(1)}_{k_1,k_2}(k_2 - k_1))(I + A^{U(1)}_{k_1,k_2}(k_2 - k_1))
\]

\[
\approx F^\dagger_{k_1,k_2} e^{2 A^{U(1)}_{k_1,k_2}(k_2 - k_1)} \quad \text{(B16)}
\]

where in the limit of \( k_2 - k_1 \ll 2\pi \) (the case in all our terms) we neglect \((k_2 - k_1)^2 \) order terms, and where \( A_{k_1,k_2} \) is the full \( U(2) \) field strength. We have also used the fact that:

\[
A^{mn}_{k_1,k_2}(k_2 - k_1) = \langle m, k_1 | (| n, k_2 \rangle - | n, k_1 \rangle)
\]

\[
= \langle m, k_1 | n, k_2 \rangle - \delta_{mn}
\]

\[
= \delta_{mn} - \langle m, k_2 | n, k_1 \rangle
\]

\[
= -[\langle n, k_1 | m, k_2 \rangle - \delta_{mn}]^*
\]

\[
= -A^{mn}_{k_2,k_1}^*(k_2 - k_1) \quad \text{(B17)}
\]

For \( k_2 - k_1 \ll 2\pi \), to give the above equation, we used the finite difference version of the equality:

\[
\langle m, k | n, k \rangle = \delta_{mn} \rightarrow (\partial_k (m,k) | n, k) + \langle m, k | (\partial_k | n, k) \rangle = 0
\]

which reads by putting:

\[
\langle \partial_k (m, k_1) | n, k_1 \rangle = \frac{\langle m, k_2 - | m, k_1 \rangle | n, k_1 \rangle}{k_2 - k_1}
\]

\[
(\partial_k (m, k_1) | n, k_1 \rangle = \frac{\langle m, k_2 - | m, k_1 \rangle | n, k_1 \rangle}{k_2 - k_1}
\]

\[
\langle m, k_2 | n, k_1 \rangle + \langle m, k_1 | n, k_2 \rangle = 2\delta_{mn} \quad \text{(B18)}
\]

After all this long detour, we have proved:

\[
F^T_{k_1,k_2} B^\dagger(0) = B^\dagger(0) F_{k_1,k_2} e^{2 A^{U(1)}_{k_1,k_2}(k_2 - k_1)} \quad \text{(B19)}
\]

We then return to the \( U(2) \) Wilson loop.

\[
D = B(N_x^2 - \Delta k) F^T_{\Delta k, -\Delta k} F^T_{\Delta k, -\Delta k} F^T_{\Delta k, -\Delta k} F^T_{\Delta k, -\Delta k} \cdots
\]

\[
\times F^T_{\Delta k, -\Delta k} F^T_{\Delta k, -\Delta k} F^T_{\Delta k, -\Delta k} F^T_{\Delta k, -\Delta k} \cdots
\]

\[
\times F^T_{\Delta k, -\Delta k} F^T_{\Delta k, -\Delta k} F^T_{\Delta k, -\Delta k} F^T_{\Delta k, -\Delta k} \cdots
\]

\[
\times F^T_{\Delta k, -\Delta k} F^T_{\Delta k, -\Delta k} F^T_{\Delta k, -\Delta k} F^T_{\Delta k, -\Delta k} \cdots
\]

\[
\times F^T_{\Delta k, -\Delta k} F^T_{\Delta k, -\Delta k} F^T_{\Delta k, -\Delta k} F^T_{\Delta k, -\Delta k} \cdots
\]

\[
\times F^T_{\Delta k, -\Delta k} F^T_{\Delta k, -\Delta k} F^T_{\Delta k, -\Delta k} F^T_{\Delta k, -\Delta k} \cdots
\]

\[
\times F^T_{\Delta k, -\Delta k} F^T_{\Delta k, -\Delta k} F^T_{\Delta k, -\Delta k} F^T_{\Delta k, -\Delta k} \cdots
\]

\[
\times F^T_{\Delta k, -\Delta k} F^T_{\Delta k, -\Delta k} F^T_{\Delta k, -\Delta k} F^T_{\Delta k, -\Delta k} \cdots
\]

\[
\times F^T_{\Delta k, -\Delta k} F^T_{\Delta k, -\Delta k} F^T_{\Delta k, -\Delta k} F^T_{\Delta k, -\Delta k} \cdots
\]

\[
\times F^T_{\Delta k, -\Delta k} F^T_{\Delta k, -\Delta k} F^T_{\Delta k, -\Delta k} F^T_{\Delta k, -\Delta k} \cdots
\]

\[
\times F^T_{\Delta k, -\Delta k} F^T_{\Delta k, -\Delta k} F^T_{\Delta k, -\Delta k} F^T_{\Delta k, -\Delta k} \cdots
\]

\[
\times F^T_{\Delta k, -\Delta k} F^T_{\Delta k, -\Delta k} F^T_{\Delta k, -\Delta k} F^T_{\Delta k, -\Delta k} \cdots
\]

\[
\times F^T_{\Delta k, -\Delta k} F^T_{\Delta k, -\Delta k} F^T_{\Delta k, -\Delta k} F^T_{\Delta k, -\Delta k} \cdots
\]

\[
\times F^T_{\Delta k, -\Delta k} F^T_{\Delta k, -\Delta k} F^T_{\Delta k, -\Delta k} F^T_{\Delta k, -\Delta k} \cdots
\]

\[
\times F^T_{\Delta k, -\Delta k} F^T_{\Delta k, -\Delta k} F^T_{\Delta k, -\Delta k} F^T_{\Delta k, -\Delta k} \cdots
\]

where we have used \( U_{0,\Delta k} U_{0,\Delta k} = U_{\Delta k, 2\Delta k} U_{\Delta k, 2\Delta k} = I, \text{ etc...} \). Hence:

\[
F^T_{k_1,k_2} B^\dagger(0) = B^\dagger(0) F_{k_1,k_2} e^{2 A^{U(1)}_{k_1,k_2}(k_2 - k_1)}
\]
\[ D = e^{2(A^{U(1)}_{\Delta k} + A^{U(1)}_{\Delta k,2\Delta k} + A^{U(1)}_{\Delta k,3\Delta k} + \cdots + A^{U(1)}_{(N_x/2-1)\Delta k,(N_x/2)\Delta k}) \Delta k} \times B(\pi)B^\dagger(0) \]  

(B21)

We note that the phase above is twice the \( U(1) \) (matrix, not traced) phase picked up from 0 to \( \pi \). Let us redefine it by re-expressing it from \( -\pi \) to \( \pi \), i.e. the full abelian Berry for the interval considered. We have

\[ A^{U(1)}_{k_1,k_2} \Delta k = \frac{1}{2} \sum_n \langle n,k_1 | (|n,k_2\rangle - |n,k_1\rangle) \]  

(B22)

\[ A^{U(1)}_{-k_2,-k_1} \Delta k = \frac{1}{2} \sum_n \langle n,-k_2 | (|n,-k_1\rangle - |n,-k_2\rangle) \]

\[ = \frac{1}{2} \sum_n \langle n,-k_2 | n,-k_1 \rangle - \langle n,-k_2 | n,-k_2 \rangle \]

\[ = \frac{1}{2} tr[F_{-k_2,-k_1} - I] \]

\[ = \frac{1}{2} tr[B(k_2)F_{k_1,k_2}B^\dagger(k_1) - I] \]  

(B23)

where we have used eq(B24). Since \( k_2 - k_1 \ll 2\pi \), we can approximate \( B(k_2) - B(k_1) \) as small and write \( B(k_2) = B(k_1) + B(k_2) - B(k_1) \) to get:

\[ A^{U(1)}_{-k_2,-k_1} \Delta k = \frac{1}{2} tr[F_{k_1,k_2}B^\dagger(k_1) - I] + (B(k_2) - B(k_1))F_{k_1,k_2}B^\dagger(k_1) \]

\[ = \frac{1}{2} tr[F_{k_1,k_2} + (B(k_2) - B(k_1))F_{k_1,k_2}B^\dagger(k_1)] \]

\[ = A^{U(1)}_{k_1,k_2} \Delta k + \frac{1}{2} tr[(B(k_2) - B(k_1))F_{k_1,k_2}B^\dagger(k_1)] \]  

(B24)

As \( B(k_2) - B(k_1) \) is considered small for \( k_2 - k_1 \ll 2\pi \), we take

\[ (B(k_2) - B(k_1))F_{k_1,k_2} \approx I \]  

if multiplied by another small number. Hence:

\[ A^{U(1)}_{-k_2,-k_1} \Delta k = A^{U(1)}_{k_1,k_2} \Delta k + \frac{1}{2} tr[(B(k_2) - B(k_1))B^\dagger(k_1)] \]  

(B26)

The first term is just the \( U(1) \) phase in the contour direction: \( \int_{-\pi}^{\pi} A^{U(1)}(k) dk \). The Wilson loop is then:

\[ W = e^{ \int_{-\pi}^{\pi} A^{U(1)}(k) dk} \]  

\[ - \frac{i}{\pi} \int_{0}^{\pi} dktr[B^\dagger(k) \nabla_k B(k)] \cdot B(\pi)B^\dagger(0) \]  

(B28)

As \( B(k) \) is unitary, we also know that:

\[ tr[B^\dagger(k) \nabla_k B(k)] = \nabla_k \log \det B(k) \]  

(B29)

and hence:

\[ e^{ - \frac{i}{\pi} \int_{0}^{\pi} dktr[B^\dagger(k) \nabla_k B(k)]} = e^{- \frac{1}{\pi} \log(\frac{\det B(\pi)}{\det B(0)})} = \sqrt{\frac{\det B(0)}{\det B(\pi)}} \]  

(B30)

The Wilson loop becomes:

\[ D = e^{ \int_{-\pi}^{\pi} A^{U(1)}(k) dk} \sqrt{\frac{\det B(0)}{\det B(\pi)}} \cdot B(\pi)B^\dagger(0) \]  

(B31)

As we said before, \( B(0), B(\pi) \) are unitary, 2 by 2 matrices, antisymmetric, so:

\[ B(0) = Pf(B(0)) \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} \]  

(B32)

\[ B(\pi) = Pf(B(\pi)) \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} \]  

(B33)

where Pf is the pfaffian of the matrix. We hence have:

\[ D = e^{ \int_{-\pi}^{\pi} A^{U(1)}(k) dk} \sqrt{\frac{\det B(0) \cdot Pf(B(\pi))}{\det B(\pi) \cdot Pf(B(0))}} \cdot I \]  

(B34)

where \( I \) is the 2 \times 2 identity matrix.

We now make several observations. Obviously, the above equality is valid on both time-reversal invariant lines at \( k_y = 0 \) and \( k_y = \pi \), i.e. we can define two Wilson loops:
\[
D(k_y = 0) = e^{i \int_{-\pi}^{\pi} A^{(1)}(k_x, k_y = 0) dk_x} \times \sqrt{\frac{\text{det} B(0, 0)}{\text{det} B(\pi, 0)}} \frac{P f(B(\pi, 0))}{P f(B(0, 0))} I
\]

and
\[
D(k_y = \pi) = e^{i \int_{-\pi}^{\pi} A^{(1)}(k_x, k_y = \pi) dk_x} \times \sqrt{\frac{\text{det} B(0, 0)}{\text{det} B(\pi, 0)}} \frac{P f(B(\pi, \pi))}{P f(B(0, \pi))} I
\]

Second, we notice that the \(U(1)\) factor phase is not just the usual abelian Berry phase but only half of it. Indeed, as per our definition:
\[
A_{k_1, k_2}^{m,n} = A_{k_1, k_2}^{U(1), i} \delta_{mn} + A_{k_1, k_2}^{SU(2), i} (\sigma^i)_{mn}
\]

This implies:
\[
A_{k}^{U(1), i} = \frac{1}{2} \sum_{m} \langle m, \vec{k} | m, \vec{k} \rangle
\]

which has a 1/2 difference from the usual form. This difference is actually important. Define:
\[
\Phi(k_y) = \int_{-\pi}^{\pi} dk_x A_x(k_x, k_y) = \log D(k_y)
\]

We then have:
\[
\int_{0}^{\pi} \nabla_{k_y} \Phi(k_y) = \int_{0}^{\pi} \nabla_{k_y} \log D(k_y) = \Phi(\pi) - \Phi(0) + 2\pi i M_n
\]

where \(M_n\) is the winding number of the phase \(\Phi(\pi)\). The phase \(\Phi(k_y)\) is the sum of the phases \(\phi_1(k_y)\) and \(\phi_2(k_y)\) of the two eigenvalues of the Wilson loop both defined in the interval \([0, 2\pi]\). Each of these eigenvalues has a winding number which adds to \(M_n\), and the system will turn to be nontrivial if the system has an odd \(M_n\). We now take the Wilson loop \(W\) from \(k_x = -\pi, \pi\) at \(k_y = 0\), and then from \(k_x = \pi, -\pi\) at \(k_y = \pi\):
\[
W = D(k_y = 0)(D(k_y = \pi))^{-1}
\]

\[
= e^{i(\Phi(\pi) - \Phi(0))} \times \sqrt{\frac{\text{det} B(0, 0)}{\text{det} B(\pi, 0)}} \frac{P f(B(\pi, 0))}{P f(B(0, \pi))} \times \sqrt{\frac{\text{det} B(0, \pi)}{\text{det} B(\pi, \pi)}} \frac{P f(B(\pi, \pi))}{P f(B(0, \pi))} I
\]

\[
= e^{i\int_{0}^{\pi} \nabla_{k_y} \log D(k_y)) + \pi i M_n} \times \sqrt{\frac{\text{det} B(0, 0)}{\text{det} B(\pi, 0)}} \frac{P f(B(\pi, 0))}{P f(B(0, \pi))} \times \sqrt{\frac{\text{det} B(0, \pi)}{\text{det} B(\pi, \pi)}} \frac{P f(B(\pi, \pi))}{P f(B(0, \pi))} I
\]

As such:
\[
D(k_y = 0) e^{i\int_{0}^{\pi} \nabla_{k_y} \log D(k_y)) + \pi i M_n} \times \sqrt{\frac{\text{det} B(0, 0)}{\text{det} B(\pi, 0)}} \frac{P f(B(\pi, 0))}{P f(B(0, \pi))} \times \sqrt{\frac{\text{det} B(0, \pi)}{\text{det} B(\pi, \pi)}} \frac{P f(B(\pi, \pi))}{P f(B(0, \pi))} I
\]

which says that the pfaffian invariant is just the parity of the band switch number \(M_n\). For \(M_n\) odd, it is nontrivial. Note that although our proof above is explicit only for two occupied bands, it can be easily extended to the \(2N_{\text{occupied}}\) band case when we realize that that case is just a tensor product (upon removing accidental degeneracies) of \(N_{\text{occupied}}\) time-reversal invariant multiplets for which the above expression applies.

Appendix C: Wilson loop and the \(Z_2\) invariant expressed as an obstruction

An alternative formulation of the \(Z_2\) invariant has been defined by Fu and Kane, where the \(Z_2\) invariant is expressed as an obstruction of the \(U(1)\) Berry’s phase gauge field in half of the Brillouin zone. This approach has some convenience in its similarity with the Chern number formula of the quantum Hall states by Thouless et al.\(^7\) The application of this approach to numerical calculation of the \(Z_2\) invariant in finite size systems has been studied by Fukui and Hatsugai\(^8\). Here we provide an alternative proof of the relation between our Wilson loop approach and the \(Z_2\) invariant through the obstruction formula. We start by reviewing the obstruction formulation of Fu and Kane (Appendix A1). Consider \([n, k]\) as the occupied Bloch bands. We make the gauge choice
\[
|n, -k\rangle = T_{nm} |m, k\rangle
\]

with \(T\) an antisymmetric matrix satisfying \(T^2 = -1\). Comparing to Eq. (B1), the gauge choice here corresponds to the requirement that \(B_{nm}(k)\) is independent from \(k\). More explicitly, with \(2N\) occupied bands we can label the bands in pairs as \([n, k]\) and \([\bar{n}, \bar{k}]\) with \(n = 1, ..., N\). Time-reversal acts as \(|\bar{n}, -k\rangle = T |n, k\rangle\), \(|n, -k\rangle = -T |\bar{n}, \bar{k}\rangle\), so that the wavefunctions in the
lower half Brillouin zone (BZ) defined by \( k_y \in [-\pi, 0] \) is determined by those in the upper half BZ, denoted by \( \tau \). With this gauge choice, for topological insulator it is not possible to make a continuous and single-valued choice of the wavefunctions in the whole Brillouin zone. However, it is always possible to define the wavefunctions continuously in the half BZ \( \tau \), so that all obstructions are pushed to the boundary between the two half BZs, i.e. the two lines \( k_y = 0 \) and \( k_y = \pi \). In such a gauge choice, Fu and Kane shows that the \( Z_\tau \) invariant is given by an obstruction in the half Brillouin zone:

\[
\Delta = \frac{1}{2\pi} \left( \oint_{\tau} A \cdot dl - \int_{\tau} d^2k F_{xy} \right) \mod 2 \tag{C2}
\]

where \( A_i = -i \sum_n \langle nk|\partial_i|nk\rangle \) is the \( U(1) \) part of the Berry phase connection. By first integrating over \( k_x \) and define the \( U \) Wilson loop

\[
\Phi(k_y) = \oint_{-\pi}^{\pi} dk_x A_x(k_x, k_y) \tag{C3}
\]

The \( Z_\tau \) invariant can be expressed as

\[
\Delta = \frac{1}{2\pi} \left( \int_{0}^{\pi} dk_y \partial_k \Phi(k_y) - (\Phi(\pi) - \Phi(0)) \right) \mod 2 \tag{C4}
\]

If we don’t have any restriction on the gauge choice (other than requiring that the wavefunctions are continuous in \( \tau \) so that \( \Phi(k_y) \) is continuous and well-defined), \( \Delta \) can be 0, or any arbitrary integer. However, the gauge choice eq.\( \text{(C4)} \) removes this ambiguity. Consider the states \( |nk\rangle \) for \( k_y = 0 \). A gauge transformation

\[
|nk\rangle \rightarrow e^{i\phi(n)}|nk\rangle \tag{C5}
\]

corresponds to a gauge transformation \( \mathbf{a} \rightarrow \mathbf{a} + \nabla k \phi \), which leads to the change in the flux

\[
\Phi(k_y = 0) \rightarrow \Phi(k_y = 0) + 2N \oint_{-\pi}^{\pi} dk_x \partial_{k_x} \phi_{k_x,0} \tag{C6}
\]

However, to preserve the condition eq.\( \text{(C1)} \) we have to require

\[
\phi_k = -\phi_{-k} \tag{C7}
\]

so that

\[
\oint_{-\pi}^{\pi} dk_x \partial_{k_x} \phi_{k_x,0} = 2 \int_{0}^{\pi} \partial_{k_x} \phi_{k_x,0} = 2 (\phi_{\pi,0} - \phi_{0,0}) \tag{C8}
\]

Since we also have \( \phi_{\pi,0} \) and \( \phi_{0,0} \) mod \( \pi \) from eq.\( \text{(C7)} \), the allowed change of \( \Phi(k_y = 0) \) in the gauge transformations that preserves the gauge choice eq.\( \text{(C1)} \) can only be

\[
\Phi(k_y = 0) \rightarrow \Phi(k_y = 0) + 4N (\phi_{\pi,0} - \phi_{0,0}) = \Phi(k_y = 0) + 4\pi n, n \in \mathbb{Z} \tag{C9}
\]

The same is true for \( \Phi(k_y = \pi) \). Consequently, \( \Phi(k_y = 0) \) and \( \Phi(k_y = \pi) \) are well-defined modular \( 4\pi \), so that the \( Z_\tau \) quantity \( \Delta \) defined by eq.\( \text{(C4)} \) is well-defined.

Now we relate this result to the non-Abelian Wilson loop. When there are \( 2N \) bands occupied, a \( U(2N) \) Berry phase gauge field \( a_{\alpha \mu}^{nm} = -i \langle nk|\partial_{\alpha}|mnk\rangle \) is defined. We can define the \( U(2N) \) Wilson loop along the same equal-\( k_y \) loops:

\[
W(k_y) = Pe^{i \oint_{-\pi}^{\pi} dk_x a_x(k_x, k_y)} \in U(2N) \tag{C10}
\]

The \( U(1) \) gauge field is related to the \( U(2N) \) gauge field by \( A_i = \text{Tr} a_i \) so that the \( U(1) \) flux \( \Phi(k_y) \) is related to \( W(k_y) \) as \( e^{i\Phi(k_y)} = \text{det} W(k_y) \). Denote the eigenvalues of \( W(k_y) \) as \( e^{i\phi_n(k_y)} \) with \( n = 1, \ldots, 2N \), we have \( \Phi(k_y) = \sum_n \phi_n(k_y) \mod 2\pi \). Thus

\[
\Delta = \frac{1}{2\pi} \sum_n \int_{0}^{\pi} dk_y \partial_{k_y} \phi_n(k_y) - \sum_n (\phi_n(\pi) - \phi_n(0)) \mod 2 \tag{C11}
\]

Now we study the effect of the gauge choice eq.\( \text{(C1)} \) on the \( U(2N) \) gauge field.

\[
a_{-k}^{nm} = -i \langle n, k|\nabla_k|m, -k\rangle = i \text{Tr}_{m} \text{Tr}_{n} T (\langle k|\nabla_k|l\rangle) \]

\[
es T_{m} T_{n} (a_{k}^{nm})* = (T a_{k}^{T} T^{-1})_{nm} \tag{C12}
\]

\[
W(-k_y) = TW(k_y) T^{-1} \tag{C13}
\]

Thus for \( k_y = 0 \) or \( \pi \), \( e^{i\phi_n(k_y)} \) is doubly degenerate. If we label a pair of degenerate eigenvalues by \( n \) and \( \bar{n} \), the gauge choice eq.\( \text{(C1)} \) corresponds to the choice of \( \phi_{n}(k_y) = \phi_{\bar{n}}(k_y) \). Indeed we see that if we make this choice, an ambiguity of \( 2\pi \) in \( \phi_n \) leads to an ambiguity of \( 4\pi \) in \( \sum_n \phi_n \). Thus \( \Delta \) defined in eq.\( \text{(C11)} \) is well-defined.

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**Figure 8:** (a) Definition of the half Brillouin zone and the paths to define Wilson loops. (b) Schematic picture of eigenvalues \( \phi_n(k_y) \) for a two band model. \( \phi_1(k_y) \) has winding number \( 0 \) and \( \phi_1(k_y) \) has winding number \( 1 \), when \( \phi_1(0) \) and \( \phi_1(\pi) \) are chosen to be in \( [0, 2\pi] \).
To simplify the formula, we choose $\phi_n(0)$ and $\phi_n(\pi)$ to be in $[0, 2\pi)$. Thus
\[
\int_0^\pi dk_y \partial_{k_y} \phi_n(k_y) = \phi_n(\pi) - \phi_n(0) + 2\pi M_n \tag{C14}
\]
with $M_n$ the winding number of phase $\phi_n$, which is equal to the number of times $\phi_n$ crosses the line $\phi = 2\pi$ from below. For example in Fig.\(\ref{fig:example}\)(b) $\phi_1$ has winding number 0 and $\phi_1$ has winding number 1. In this way we get
\[
\Delta = \sum_n M_n \mod 2 \tag{C15}
\]

The number $\sum_n M_n$ simply counts how many eigenvalues $\phi_n$ crosses $\phi = 2\pi$ line (or any other reference line) from below. Thus the $Z_2$ invariant is simply determined by the parity of the number of eigenvalue curves $\phi_n(k_y)$ which crosses a reference line $\phi = \text{constant}$.

1. R. B. Laughlin, Phys. Rev. B 23, 5632 (1981).
2. D. J. Thouless, M. Kohmoto, M. P. Nightingale, and M. den Nijs, Phys. Rev. Lett. 49, 405 (1982).
3. C. L. Kane and E. J. Mele, Phys. Rev. Lett. 95, 226801 (2005).
4. C. L. Kane and E. J. Mele, Phys. Rev. Lett. 95, 146802 (2005).
5. J. E. Moore and L. Balents, Phys. Rev. B 75, 121306 (2007).
6. R. Roy, Phys. Rev. B 79, 195322 (2009).
7. L. Fu and C. L. Kane, Phys. Rev. B 74, 195312 (2006).
8. B. A. Bernevig and S. Zhang, Phys. Rev. Lett. 96, 106802 (2006).
9. C. Wu, B. A. Bernevig, and S. Zhang, Phys. Rev. Lett. 96, 106401 (2006).
10. C. Xu and J. E. Moore, Phys. Rev. B 73, 045322 (2006).
11. A. Roth, C. Brune, H. Buhmann, L. W. Molenkamp, J. Maciejko, X. Qi, and S. Zhang, Science 325, 294 (2009).
12. M. Konig, S. Wiedmann, C. Brune, A. Roth, H. Buhmann, L. W. Molenkamp, X. Qi, and S. Zhang, Science 318, 766 (2007).
13. B. A. Bernevig, T. L. Hughes, and S. Zhang, Science 314, 1757 (2006).
14. X. Qi, Y. Wu, and S. Zhang, Phys. Rev. B 74, 085308 (2006).
15. L. Fu, C. L. Kane, and E. J. Mele, Phys. Rev. Lett. 98, 106803 (2007).
16. L. Fu and C. L. Kane, Phys. Rev. B 76, 045302 (2007).n
17. J. C. Y. Teo, L. Fu, and C. L. Kane, Phys. Rev. B 78, 045426 (2008).
18. T. Fukui and Y. Hatsugai, J. Phys. Soc. Jpn. 76, 053702 (2007).
19. Y. Ran, Y. Zhang, and A. Vishwanath, Nature Phys. 5, 298 (2009).
20. H. Zhang, C. Liu, X. Qi, X. Dai, Z. Fang, and S. Zhang, Nat Phys 5, 438 (2009).
21. Y. L. Chen, J. G. Analytis, J. Chu, Z. K. Liu, S. Mo, X. L. Qi, H. J. Zhang, D. H. Lu, X. Dai, Z. Fang, et al., Science 325, 178 (2009).
22. D. Hsieh, D. Qian, L. Wray, Y. Xia, Y. S. Hor, R. J. Cava, and M. Z. Hasan, Nature 452, 970 (2008).
23. Y. Xia, D. Qian, D. Hsieh, L. Wray, A. Pal, H. Lin, A. Bansil, D. Grauer, Y. S. Hor, R. J. Cava, et al., Nat Phys 5, 308 (2009).
24. J. G. Analytis, J. Chu, Y. Chen, F. Corredor, R. D. McDonald, Z. X. Shen, and I. R. Fisher, Phys. Rev. B 81, 205407 (2010).
25. D. Hsieh, Y. Xia, D. Qian, L. Wray, F. Meier, J. H. Dil, J. Osterwalder, L. Patthey, A. V. Fedorov, H. Lin, et al., Phys. Rev. Lett. 103, 146401 (2009).
26. S. R. Park, W. S. Jung, C. Kim, D. J. Song, C. Kim, S. Kimura, K. D. Lee, and N. Hur, Phys. Rev. B 81, 041405 (2010).
27. S. Shen, e-print arXiv:0909.4125 (2009).
28. B. Yan, C. Liu, H. Zhang, C. Yam, X. Qi, T. Frauenheim, and S. Zhang, EPL (Europhysics Letters) 90, 37002 (2010).
29. H. Lin, L. A. Wray, Y. Xia, S. Xu, S. Jia, R. J. Cava, A. Bansil, and M. Z. Hasan, Nat Mater 9, 546 (2010).
30. M. Z. Hasan and C. L. Kane, e-print arXiv:1002.3895 (2010).
31. W. Shan, H. Lu, and S. Shen, New J. Phys. 12, 043048 (2010).
32. P. Roushan, J. Seo, C. V. Parker, Y. S. Hor, D. Hsieh, D. Qian, A. Richardella, M. Z. Hasan, R. J. Cava, and A. Yazdani, Nature 460, 1106 (2009).
33. Z. Alpichshev, J. G. Analytis, J. H. Chu, I. R. Fisher, and A. Kapitulnik, e-print arXiv:1003.2233 (2010).
34. W. Lee, C. Wu, D. P. Arovas, and S. Zhang, Phys. Rev. B 80, 245439 (2009).
35. Y. Zhang, K. He, C. Chang, C. Song, L. Wang, X. Chen, J. Jia, Z. Fang, X. Dai, W. Shan, et al., Nat Phys 6, 584 (2010).
36. T. Zhang, P. Cheng, X. Chen, J. Jia, X. Ma, K. He, L. Wang, H. Zhang, X. Dai, Z. Fang, et al., Phys. Rev. Lett. 103, 266803 (2009).
37. X. Zhou, C. Fang, W. Tsai, and J. Hu, Phys. Rev. B 80, 245317 (2009).
38. H. Guo and M. Franz, Phys. Rev. B 81, 041102 (2010).
39. D. Hsieh, Y. Xia, D. Qian, L. Wray, J. H. Dil, F. Meier, J. Osterwalder, L. Patthey, J. G. Checkelsky, N. P. Ong, et al., Nature 460, 1101 (2009).
40. D. Hsieh, Y. Xia, L. Wray, D. Qian, A. Pal, J. H. Dil, J. Osterwalder, F. Meier, G. Bihlmayer, C. L. Kane, et al., Science 323, 919 (2009).
41. T. Fukui, Y. Hatsugai, and H. Suzuki, J. Phys. Soc. Jpn. 74, 1674 (2005).
42. R. D. King-Smith and D. Vanderbilt, Phys. Rev. B 47, 1651 (1993).
43. J. D. Thouless, Phys. Rev. B 27, 6083 (1983).
44. X. Dai, T. L. Hughes, X. Qi, Z. Fang, and S. Zhang, Phys. Rev. B 77, 125319 (2008).
45. A. Kobayashi, O. F. Sankey, and J. D. Dow, Phys. Rev. B 25, 6367 (1982).
46 C. Liu, H. Zhang, B. Yan, X. Qi, T. Frauenheim, X. Dai, Z. Fang, and S. Zhang, Phys. Rev. B 81, 041307 (2010).
47 W. Zhang, R. Yu, H. Zhang, X. Dai, and Z. Fang, New Journal of Physics 12, 065013 (2010), ISSN 1367-2630.
48 S. Murakami, Phys. Rev. Lett. 97, 236805 (2006).
49 Y. Liu and R. E. Allen, Phys. Rev. B 52, 1566 (1995).
50 A. A. Soluyanov and D. Vanderbilt, e-print arXiv:1009.1415 (2010).