A $\mathbb{Z}_2$ index of a Dirac operator with time reversal symmetry

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Abstract

With time reversal symmetry a Dirac operator has a vanishing index and a Chern number. We show that we can nevertheless define a nontrivial $\mathbb{Z}_2$ index as well as a corresponding topological invariant given by gauge field, which implies that such a Dirac operator is topologically nontrivial.

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The idea of topological invariants has been successfully applied to various fields in physics. In gauge theories they are used to classify topological configurations such as monopoles and instantons. When couplings with chiral fermions are introduced, there arise interesting field theoretical phenomena such as chiral anomaly and gauge anomaly [1]. The chiral anomaly [1] is known to have an intimate relationship with the index theorem [2] which tells us that the index of the Dirac operator coincides with the second Chern number. The gauge anomaly also has a topological origin, since it is related to the chiral anomaly in six dimensions [3].

In condensed matter physics, it is well known that the plateaus of the quantum Hall effect (QHE) are classified by the first Chern number [4, 5]. Recently, a novel topological number has been proposed by Kane, Mele and Fu [6–8] for the quantum spin Hall effect (QSHE) [6–9]. It is invariant only modulo 2, and is often called the $\mathbb{Z}_2$ invariant. Here, time reversal symmetry is the key difference between the QHE and the QSHE. Remarkably, the QSHE has recently been observed in several experiments [10–13].

The formula of the $\mathbb{Z}_2$ invariant proposed by Fu and Kane [8] is, roughly speaking, ‘half’ the first Chern number. Therefore, it is very useful [14] for numerical calculations if we utilize the techniques of computing the Chern number in the lattice gauge theories [15]. Besides such practical applications, it is of fundamental importance, since it could be a topological invariant in ‘mod 2 index theorem’ [16]. Therefore, if we find a corresponding analytical invariant, we can obtain a simple formula of a $\mathbb{Z}_2$ index theorem for a (pseudo-real) Dirac operator.

In this paper, we investigate analytical and topological invariants associated with a Dirac operator with time reversal invariance. We first study its spectral properties in Euclidean space and define a $\mathbb{Z}_2$ index of the Dirac operator. We then propose a topological invariant which is a generalization of the Fu–Kane formula, and infer that it coincides with the $\mathbb{Z}_2$ index.
We begin by recalling the time reversal transformation of Dirac fermions in \( d = 2n + 2 \) (\( n = 0, 1, \ldots \)) dimensional Minkowski space time. It is defined by \( \psi(t, x) \rightarrow T \psi(-t, x) \), where \( T \) is an anti-unitary operator, \( T \equiv \Gamma_5 \Gamma_0 \), with \( \Gamma_\nu \) being a product of some \( \gamma \) matrices, \( \Gamma_5 \) a generator of a gauge group \( G \), and \( \Gamma_0 \) the operator of taking complex conjugate.

For the Lagrangian density \( \mathcal{L}(t, x) = \bar{\psi}(t, x) i \mathcal{D}(t, x) \psi(t, x) \) to transform as \( \mathcal{L}(t, x) \rightarrow \mathcal{L}(-t, x) \) under time reversal, we see that \( i \mathcal{D}(t, x) T^{-1} = i \bar{\mathcal{D}}(-t, x) \), from which it follows that

\[
T \gamma^\mu T^{-1} = \gamma_\mu, \quad T A_\mu(t, x) T^{-1} = A^\mu(-t, x),
\]

where the metric is \( g_{\mu\nu} = \text{diag}(1, -1, \ldots, -1) \). The \( \Gamma_5 \) matrix anti-commuting with the Dirac operator is given by \( \Gamma_5 = i^{d/2-1} \gamma^0 \gamma^1 \cdots \gamma^{d-1} \). This definition directly leads to \( TT_5 T^{-1} = -I_5 \) for \( d = 4n + 2 \) and \( = +I_5 \) for \( d = 4n + 4 \).

\( T \) has the following two possibilities: \( T^2 = \pm 1 \), depending on \( \Gamma_5 = \pm 1 \) and \( \Gamma_5^2 = \pm 1 \). The former is determined solely by the space-time dimension \( d \); in \( d = 2 \), for example, we can choose \( \gamma^0 = \sigma_2 \) and \( \gamma^1 = i \sigma_1 \). Since these are imaginary, \( K(\gamma^0, \gamma^1) K^{-1} = (\gamma^0, -\gamma^1) \), we see that \( T \gamma = -i \gamma^1 = \sigma_1 \), and therefore, \( \Gamma_5^2 = 1 \). In general, we have \( \Gamma_5^2 = 1 \) for \( d = 0, 2 + 8n \), and \( \Gamma_5^2 = -1 \) for \( d = 4, 6 + 8n \).

To discuss the index of the Dirac operator with time reversal invariance, we switch from Minkowski space to Euclidean space. It is defined by rotating all the spatial coordinates \( x^j (j = 1, \ldots, d-1) \) onto the imaginary axes via \( x^j = i y^j \), whereas \( x^0 = y^d \). As we shall see, this enables us to relate a \( Z_2 \) index of the Dirac operator with a topological invariant.

The metric becomes in this case \( g_{\mu\nu} = \delta_{\mu\nu} \). Correspondingly, the \( \gamma \) matrices are introduced via \( \gamma^j = i \gamma^j \) and \( \gamma^0 = \gamma^d \) which become Hermitian \( \gamma^j = \gamma^j \), and the gauge potential \( A_\mu(x) \) via \( A_j(x) = -i A_j(x) \) and \( A_0(x) = A_d(x) \). Then, the Dirac operator can be denoted as \( i \mathcal{D}(x) = i \mathcal{D}(y) \equiv i \gamma^\mu (\partial^\mu - i A(x)) \) which we regard as Hermitian \( (i \mathcal{D}(y))^\dagger = i \mathcal{D}(y) \).

The transformation law under time reversal becomes

\[
T \gamma^\mu T^{-1} = \gamma^\mu, \quad T A_\mu(y) T^{-1} = A_\mu(-y),
\]

which follows from the same transformation law (1) but with the Euclidean metric mentioned above. Therefore, the Dirac operator transforms as

\[
T i \mathcal{D}(y) T^{-1} = i \mathcal{D}(-y).
\]

Note that this transformation is for a flat space: if we consider a curved space, it should be modified suitably, as we shall see. Other key symmetry is chiral symmetry described by

\[
\Gamma_5 i \mathcal{D}(y) + i \mathcal{D}(y) \Gamma_5 = 0.
\]

The \( Z_2 \) index discussed in this paper is involved in the case with both of the conditions

\[
T^2 = -1, \quad T \Gamma_5 T^{-1} = -\Gamma_5
\]

Intrinsic topological nature of the system can also be proved in Minkowski space like spectral flow and chiral anomaly. However, their topological characterization can be best achieved in Euclidean space compactified by suitable boundary conditions.

Even in conventional imaginary-time Euclidean space, we can also define a \( Z_2 \) index of the Dirac operator similarly in the text: time reversal invariance is given by \( T \mathcal{D}(x) T^{-1} = -\mathcal{D}(x) \), where \( \mathcal{D}(x) \) is the Hermitian Dirac operator and \( x \) denotes the coordinates of imaginary-time Euclidean space. By the use of the anti-commutativity of \( \mathcal{D} \) and \( \Gamma_5 \), we see that a similar discussion of the quartet formation at nonzero energies can apply. However, in this case, it is not possible, as far as we study, to find a corresponding topological invariant.
fulfilled. The former ensures that the eigenstates are always doubly degenerate, which is referred to as the Kramers doublet. The latter claims that the zero-mode Kramers doublet have opposite chiralities. These conditions give some constraints: equation (5b) is valid only in $d = 4n + 2$, and equation (5a) imposes $\Gamma_G^2 = -1$ for $d = 8n + 2$ and $\Gamma_G^2 = 1$ for $d = 8n + 6$. Typical example in the former case is $\Gamma_G = 1_N \otimes \tau_2 \equiv J_2$, whereas in the latter case, a convenient but nontrivial choice may be $\Gamma_G = 1_N \otimes \tau_1 \equiv J_1$, provided that the dimension of the representation of the gauge group G is $2N$. The transformation law of gauge potentials is thus defined by

$$
A_\mu(-y) = \begin{cases}
J_2A_\mu^+(y)J_2^{-1} & \text{for } d = 8n + 2 \\
J_1A_\mu^+(y)J_1^{-1} & \text{for } d = 8n + 6
\end{cases}
$$

For a time reversal invariant Dirac operator discussed so far, we shall define a Z_2 index. Let $\psi_k(y)$ be an eigenstate of $i\hat{D}$:

$$i\hat{D}(y)\psi_k(y) = \varepsilon_k\psi_k(y).$$

Then, equation (3) ensures that $\psi_{k\bar{k}}(y) \equiv T\psi_{k\bar{k}}(-y)$ is also an eigenstate of $i\hat{D}(y)$ with the same eigenvalue $\varepsilon_k$. Here, condition (5a) plays a vital role in the orthogonality between $\psi_k$ and $\psi_{k\bar{k}}$. It thus turns out that all eigenstates are doubly degenerate, called Kramers doublets as mentioned above, which we denote as $\Phi_k(y) = (\psi_k(y), \psi_{k\bar{k}}(y))$. The spectrum is illustrated in figure 1.

Let us concentrate on the zero-mode eigenstates, $\Phi_{0,\alpha}$ ($\alpha = 1, \ldots, N_K$). Since the Dirac operator anti-commutes with $\Gamma_5$, the zero modes can be chosen to be eigenstates of the chirality. Suppose $\Gamma_5\psi_{0,\alpha} = +\psi_{0,\alpha}$. Then, we see $\Gamma_5\psi_{k\bar{0},\alpha} = -\psi_{k\bar{0},\alpha}$ because of equation (5b). Namely, at the zero energy, each Kramers doublet is composed of two states with opposite

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3 This choice of $J_1$ is just for a practical reason: it allows us to give a nontrivial example of models by the use of equation (9). As far as symmetry is concerned, we can choose $J_1 = 1$. (See footnote 5).

4 In the $d = 8n + 6$ case, odd-dimensional representations may be possible. However, for simplicity, we assume that the dimension is even, since it enables us to have nontrivial models that belong to the nontrivial element of $Z_2$, as we shall see momentarily.
Figure 2. An example of a two-dimensional manifold $M$. $y_j$ denotes the time reversal invariant points. The square represents $S^2$ if the boundary is regarded as one point. In this case, time reversal invariant points are just two, $y_1$ and $y_2 (= y_3 = y_4)$. If the two parallel boundaries are pasted and the periodic boundary conditions are imposed on each direction, the same square now denotes $T^2$, which has four time reversal invariant points.

chiralities. Even when there are some doublets at the zero energy, the number of states with positive chirality is the same as the number of states with negative chirality:

$$\text{ind } \mathcal{iD} = \dim \ker \mathcal{iD}_+ - \dim \ker \mathcal{iD}_- = 0,$$

where $\mathcal{iD}_\pm = \mathcal{iD} P\pm$ with $P\pm \equiv (1 \pm \Gamma_5)/2$. The index of the present Dirac operator is thus trivial. Nevertheless, the time reversal invariance (3), if combined with chiral symmetry (4), gives an interesting invariant. Chiral symmetry (4) tells that if $\Phi_k$ is an eigen-doublet with the energy $\varepsilon_k$, the state defined by $\Phi^\dagger \Gamma^5 \Phi_k$ is also an eigen-doublet with the opposite energy $-\varepsilon_k$. Therefore, nonzero-mode states form a quartet in this sense. Suppose that we have just one Kramers doublet at the zero energy. Then, it turns out that this doublet is stable against perturbations with time reversal and chiral symmetries, since these two states cannot move to nonzero energies without two more states in order to ensure both the symmetries. On the other hand, if there are two doublets at the zero energy, they are not obliged to stay there: small perturbations enable two of them to move to the positive energies and the other two to move to the opposite negative energies. In more general, we can claim that evenness or oddness of the number of the zero-mode Kramers doublets is an analytic invariant, from which we define a $\mathbb{Z}_2$ index of the Dirac operator with time reversal symmetry,

$$\text{ind } \mathcal{iD} = \dim \ker \mathcal{iD} \mod 2.$$  

Next, we define a topological invariant given by the gauge field. To this end, we must first specify the manifold compatible with the condition (3). Let $M$ be a compact manifold without boundary. We assume that it can be divided into two $M\pm$ such that if $y \in M_+$, $-y \in M_-$. For the time reversal invariant points $y_j = -y_j$ ($j = 1, \ldots, N_{\text{inv}}$). The number $N_{\text{inv}}$ of such points depends on $M$. For example, the 2-sphere $S^2$ has two invariant points, whereas the 2-torus $T^2$ has four invariant points, as illustrated in figure 2.

To define a topological invariant, it is convenient to define a gauge potential 1-form $A = -iA_\mu dy^\mu$ and the corresponding field strength 2-form $F = dA + A^2$. Time reversal invariance (2) or (6) tells that the Chern number $C_d$ ($d = 4n + 2$ with $n = 0, 1, \ldots$) vanishes:

$$C_d = \mathcal{N}_d/2 \int_M \text{tr } F^{d/2} = 0,$$

where the numerical factor is $\mathcal{N}_d \equiv i^n/[n!(2\pi)^n]$. This is consistent with the spectral property of the Dirac operator whose index is zero, as discussed above. This feature is quite similar to the QSHE: the first Chern number associated with the Berry phase in the Brillouin
zone \((T^2)\) vanishes due to time reversal symmetry. Nevertheless, the QSHE phase is the topologically nontrivial phase which can be described by the \(Z_2\) number, as shown by Kane et al [7, 8]. Motivated by their work, we propose that the \(Z_2\) index \((7)\) in \(d = 4n + 2\) is equivalent to

\[
D_d = \mathcal{N}_{d/2} \left[ \int_{\partial M_+} \mathrm{tr} \mathcal{F}^{d/2} - \int_{\partial M_-} \omega_{d-1}(A) \right].
\]  

(8)

mod 2. Here, \(\omega_{d-1}\) is the Chern–Simons \((d - 1)\)-form which obeys \(\mathrm{tr} \mathcal{F}^{d/2} = d \omega_{d-1}(A)\) [17]. It should be noted that formula \((8)\) has meaning under condition \((6)\). This is the reason we have adopted an unconventional Wick rotation (see footnote 2).

We must first examine the gauge dependence of \(D_d\). Let \(A_g = g^{-1} A g + g^{-1} \mathrm{dg}\) be the gauge transform of \(A\). If the time reversal invariance \((6)\) is enforced on \(A_g\), \(g\) should obey \(g(-y) = J_2 g^*(y) J_2^{-1}\) for \(d = 8n + 2\) or \(g(-y) = J_1 g^*(y) J_1^{-1}\) for \(d = 8n + 6\). We will refer to this condition as the time-reversal constraint on the gauge transformation. Let \(\Delta_{d-1}[g] \equiv D_d[A_g] - D_d[A]\) be the gauge dependence of \(D_d\). Note

\[
\omega_{d-1}(A_g) - \omega_{d-1}(A) = \omega_{d-1}(g^{-1} \mathrm{dg}) + d \alpha_{d-2},
\]

where \(\alpha_{d-2}\) is a \((d - 2)\)-form [17], which leads to

\[
\Delta_{d-1}[g] = \frac{(-1)^{n+1} (2n)!}{(2\pi)^{d+2}} \int_{\partial M_+} \mathrm{tr}(g^{-1} \mathrm{dg})^{2n+1},
\]

where \(d = 4n + 2\). Let us estimate the above in the case of \(M = S^d\) \((\partial M_+ = S^{d-1})\) for simplicity. Note that generic \(U(2N)\) gauge transformation \(g\) can be decomposed into \(U(1) \times \mathrm{SU}(2N)\) such that \(g(y) = e^{i\phi(y)} \tilde{g}(y)\) where det \(\tilde{g} = 1\). The time reversal constraint tells that \(\phi(-y) = -\phi(y)\) mod \(2\pi\). In \(d = 2\) (i.e., \(n = 0\)), \(\Delta_1[g]\) is given by this \(U(1)\) part, \(\Delta_1[g] = -N/\pi \int \mathrm{d} \phi\), where line integral is over \(S^1\), namely, the equator of \(S^2\). This gives manifestly an even integer. On the other hand, in higher dimensions, contribution from \(U(1)\) vanishes and only the non-Abelian sector \(\tilde{g}\) enters into \(\Delta_{d-1}\); \(\Delta_{d-1}[g] = \Delta_{d-1}[\tilde{g}]\). The time reversal constraint tells that at the time reversal invariant points \(y_j\) \((j = 1, 2, \text{on } S^{d-1})\), \(\tilde{g}(y_j) \equiv h(y_j) \in \mathrm{Sp}(N)\) for \(d = 8n + 2\), whereas \(h(y_j) \in \mathrm{O}(2N)\) for \(d = 8n + 6\). First, let us consider the former case. Assume that \(\tilde{g}\) takes \(\tilde{g}_0 \notin \mathrm{Sp}(2N)\) at a certain \(y, \tilde{g}(y) = \tilde{g}_0\). Then, \(y\) cannot be \(y_j\), and the time reversal constraint ensures that at \(\tilde{g}(y) = \tilde{g}_0\). There are thus an even number of points on \(S^{d-1}\) which are mapped to \(\tilde{g}_0\). It turns out that the degree of the map \(\tilde{g}\) is even, implying that the winding number, \(\Delta_{d-1}[\tilde{g}]\), is even. On the other hand, if one cannot find any \(\tilde{g}_0 \notin \mathrm{Sp}(N)\) on \(S^{d-1}\), namely, if \(\tilde{g}(y) \in \mathrm{Sp}(N)\) for all \(y\), \(\Delta_{d-1}[\tilde{g}] = 0\). We thus conclude that \(\Delta_{d-1}[g]\) is an even integer for \(d = 8n + 2\). The case \(d = 8n + 6\) \((n = 0, 1, \ldots)\) is likewise.

If the gauge potential can be smooth on the whole \(M_+\), \(D_d\) should be zero, which is a trivial element of \(Z_2\). Now we shall show that there exists not only such a trivial element but also a nontrivial element indeed. We assume that the \(u(2N)\) gauge potential is \(2 \times 2\) block-diagonal. Then, the time reversal invariance \((6)\) requires that the upper and lower \(u(N)\) sectors of the gauge potential are not independent, given generically by the form

\[
A_\mu(y) = \begin{pmatrix} a_\mu(y) & 0 \\ 0 & a_\mu^*(\tau(y) \equiv -y) \end{pmatrix},
\]

(9)

where \(a_\mu(y)\) denotes a \(u(N)\) gauge potential. In this block-diagonal case, since the upper and lower sectors are decoupled, the \(Z_2\) index and \(D_d\) can be separately computed such that

\footnote{In a suitable basis, \(\tau^1\) becomes diagonal \(\tau^1\). Then, we see \(h \in \mathrm{O}(N, N, C) \simeq \mathrm{O}(2N, C)\). It thus turns out \(\mathrm{O}(2N, C) \cap \mathrm{SU}(2N) = \mathrm{O}(2N)\).}
Consider a Dirac operator on $S^2$ in magnetic monopole background fields \cite{18}, and the north poles, respectively. From equation (9) it follows that the lower potential should be $a(\mu(y))$ and that the upper sector is nontrivial, which yields a nonzero index and the Chern number. This means that $a_\mu(y)$ cannot be smooth over $S^2$: For simplicity, assume that we have two kinds of gauge such that $a(\mu(y))$ is regular in $M_+$, collecting all singularities in $M_+$. The ordinary index theorem \cite{6} claims that ind $i\mathcal{D}_\uparrow = N_+ - N_-$, where $N_\pm$ is the number of the zero-mode with the chirality $\pm$. Now let us choose $a(\mu(y))$ as the upper gauge potential. Then, equation (8) gives $D_{d\uparrow} = \text{ind} i\mathcal{D}_\uparrow = N_+ - N_-$, since in this case, $a(\mu(y))$ is regular in $M_-$ and therefore,

\[
-\int_{\partial M_\pm} \omega_{d-1}(A) = \int_{\partial M_-} \omega_{d-1}(A) = \int_{M_-} \text{tr} \mathcal{F}^{d/2}
\]

holds if the lower gauge potential is neglected. Next, let us switch to the case with a lower gauge potential only, which should be $a(\mu(y)) = (-y)$. Since this gauge potential is regular in $M_+$, it never contributes to equation (8); $D_{d\downarrow} = 0$. It thus turns out that $D_\pm = N_+ - N_-$ holds for the full gauge potential $A_\mu$ in equation (9). On the other hand, since $i\mathcal{D}_\downarrow$ has $N_\mp$ zero-mode with chirality $\pm$, i.e., \text{ind} $i\mathcal{D}_\downarrow = N_+ - N_-$ (see footnote 6), we reach \text{ind} $i\mathcal{D}_\downarrow = N_+ + N_-$. Therefore, we conclude that \text{ind} $i\mathcal{D}_\downarrow = D_{d\downarrow} \mod 2$.

Let us now take into account off-diagonal elements of the gauge potential. The singularities in the upper gauge potential may move but stay in $M_+$ if off-diagonal elements are small enough. Even if one of them moves into $M_-$, its partner in the lower gauge potential in $M_-$ moves into $M_+$. This is due to equation (6) which ensures that if $A_\mu$ has a singularity at $y$, an opposite singularity appears at $-y$. Therefore, $D_\pm$ can change only by 2. On the other hand, along the change of the gauge potential, the spectrum of the Dirac operator flows, and a nonzero-mode quartet can be two zero-mode doublets and vice versa, which result in the change of the $\mathbb{Z}_2$ index also by 2. From the point of view of such moving singularities, the mod 2 gauge dependence of $D_\pm$ can be understood likewise. It thus turns out that $D_\pm$ and the $\mathbb{Z}_2$ index change by 2 and therefore coincide mod 2.

Finally, we shall exemplify a Dirac operator with a nontrivial $\mathbb{Z}_2$ index in $d = 2$. Let us consider a Dirac operator on $S^2$ in magnetic monopole background fields \cite{18},

\[
i\mathcal{D}(\theta, \phi) = i\sigma^1 \left( \partial_\theta + \frac{1}{2} \cot \theta - iA_\theta \right) + \frac{i\sigma^2}{\sin \theta} (\partial_\phi - iA_\phi),
\]

where $0 \leq \theta \leq \pi$ and $-\pi \leq \phi \leq \pi$ are polar coordinates, $A_\theta$ and $A_\phi$ are u(2) gauge potentials of the type (9), and the cotangent term is due to the spin connection \cite{18}. This Dirac operator has time reversal symmetry

\[
T i\mathcal{D}(\theta, \phi) T^{-1} = i\mathcal{D}(\pi - \theta, -\phi),
\]

where $T = \sigma^1 i\text{tr}^2 \mathcal{K}$. Two time reversal invariant points are $(\theta, \phi) = (\pi/2, 0)$ and $(\pi/2, \pi)$. For the upper gauge potential we have two well-known possibilities,

\[
a_\phi(\pm)(\theta) = \frac{m}{2} (\pm 1 - \cos \theta),
\]

and $a_\theta = 0$, where $a_\phi^{(\pm)}$ is the charge-$m$ monopole potential with a singularity at the south and the north poles, respectively. From equation (9) it follows that the lower potential should be $a_\phi(\pm)(\pi - \theta) = -a_\phi^{(\mp)}(\theta)$, telling that it denotes a monopole with the opposite charge and with the singularity at the opposite pole.

Assume $m \geq 0$ and choose $a_\phi^{(+)}$ as the upper gauge potential. Then, $i\mathcal{D}_\uparrow$ gives just $m$ zero modes with chirality $+$, whereas $i\mathcal{D}_\downarrow$ gives the same $m$ zero modes but with chirality $-$.\footnote{Note that $i\mathcal{D}_\uparrow$ is not invariant under time reversal: it obeys $T i\mathcal{D}_\uparrow(y) T^{-1} = i\mathcal{D}_\downarrow(y)$.}
On the other hand, we see $D_{d_1}^+ = m$ and $D_{d_1}^- = 0$. Therefore, for this decoupled model and the present gauge fixing, the $Z_2$ index and $D_2$ coincide, $\text{ind}_p i D = m = D_2$. However, as discussed, these can change by 2 by gauge transformations and/or deformation of the gauge potential, and generically coincide modulo 2.

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