Fu-Kane $\mathbb{Z}_2$ topological invariant

Kohei Kawabata (Institute for Solid State Physics, University of Tokyo)

22nd December 2024

We investigate time-reversal-invariant $2N$-band insulators in two dimensions in class AII:

$$\mathcal{T} H(\boldsymbol{k}) \mathcal{T}^{-1} = H(-\boldsymbol{k}), \quad \mathcal{T}^2 = -1 \tag{1}$$

with an antiunitary operator $\mathcal{T}$ (i.e., $\mathcal{T}\mathcal{T}^\dagger = \mathcal{T}^\dagger \mathcal{T} = 1$, $\forall z \in \mathbb{C}$ $\mathcal{T} z \mathcal{T}^{-1} = z^*$). While time-reversal symmetry enforces the vanishing of the Chern number, it gives rise to a $\mathbb{Z}_2$ topological invariant. Here, we formulate this $\mathbb{Z}_2$ topological invariant following Ref. [1]. The Chern number can be characterized as a pump of the charge polarization. Similarly, we first introduce a time-reversal-invariant counterpart of the polarization, denoted by time-reversal polarization in Ref. [1], and formulate the $\mathbb{Z}_2$ topological invariant as its spin pump[*1]. As a basic strategy, we consider the band structure protected by time-reversal symmetry, particularly focusing on half of the bands (i.e., half of the Kramers pairs) in the entire Brillouin zone, or equivalently, all the bands in half of the Brillouin zone.

1 Time-reversal polarization

We first consider a one-dimensional $2N$-band insulator $H(k)$ that respects time-reversal symmetry in Eq. (1) and introduce its time-reversal polarization. Owing to time-reversal symmetry in Eq. (1), eigenstates generally exhibit Kramers degeneracy, represented as[*2]

$$|u_n^{\mathrm{I}}(-k)\rangle = -e^{\mathrm{i}\chi_n(k)} \mathcal{T} |u_n^{\mathrm{II}}(k)\rangle, \quad |u_n^{\mathrm{II}}(-k)\rangle = e^{\mathrm{i}\chi_n(-k)} \mathcal{T} |u_n^{\mathrm{I}}(k)\rangle \tag{2}$$

with a gauge $\chi_n \in \mathbb{R}$. For each $s \in \{\mathrm{I}, \mathrm{II}\}$, we define the Berry connection as

$$A^s(k) \coloneqq \mathrm{i} \sum_n \langle u_n^s(k) | \partial_k | u_n^s(k) \rangle, \tag{3}$$

and the polarization as

$$P^s \coloneqq \oint_{-\pi}^{\pi} \frac{dk}{2\pi} A^s(k). \tag{4}$$

While the polarization P^s for one of the Kramers pairs may appear to depend on the specific choice of the labels I and II, we below demonstrate that this is not the case: P^s is invariant with respect to the choice of these labels I and II. We further show that its difference $P_\theta \coloneqq P^{\mathrm{I}} - P^{\mathrm{II}}$, referred to as the time-reversal polarization in Ref. [1], satisfies[*3]

[*1] The conceptual significance of a $\mathbb{Z}_2$ "$\mathcal{T}$ polarization" was already noted in Ref. [2], although its precise formulation was provided in Ref. [1].

[*2] We assume no degeneracy other than the Kramers degeneracy.

[*3] For an antisymmetric matrix $A = \begin{pmatrix} 0 & a \\ -a^T & 0 \end{pmatrix}$ with an $n \times n$ matrix a, its Pfaffian reads $\mathrm{Pf}\,A = (-1)^{n(n-1)/2}\,a$. We generally have $\det A = (\mathrm{Pf}\,A)^2$ and $\mathrm{Pf}\left(BAB^T\right) = (\mathrm{Pf}\,A)(\det B)$ for an arbitrary matrix B.

$$(-1)^{P_\theta} = \frac{\mathrm{Pf}\, w(0)}{\sqrt{\det w(0)}} \frac{\mathrm{Pf}\, w(\pi)}{\sqrt{\det w(\pi)}}, \tag{5}$$

with[*4]

$$w_{mn}(k) := \langle u_m(-k)|\mathcal{T}|u_n(k)\rangle. \tag{9}$$

Here, the branches of $\pm\sqrt{\det w(k)}$ are chosen to ensure that the branch at $k=0$ is continuously connected to that at $k=\pi$.

We begin with

$$A^{\mathrm{I}}(-k) = \mathrm{i}\sum_n \langle u_n^{\mathrm{I}}(-k)|\partial_k|u_n^{\mathrm{I}}(-k)\rangle = A^{\mathrm{II}}(k) - \sum_n \partial_k\chi_n(k), \tag{10}$$

and hence have

$$P^{\mathrm{I}} = \int_0^\pi \frac{dk}{2\pi}\left[A^{\mathrm{I}}(k) + A^{\mathrm{I}}(-k)\right] = \frac{1}{2\pi}\left[\int_0^\pi dk\, A(k) - \sum_n\left[\chi_n(\pi) - \chi_n(0)\right]\right] \tag{11}$$

with the total Berry connection $A := A^{\mathrm{I}} + A^{\mathrm{II}}$. Meanwhile, w introduced in Eq. (9) reduces to

$$\begin{aligned} w(k) &= \sum_n 1_{n,n}\otimes\begin{pmatrix}\langle u_n^{\mathrm{I}}(-k)|\mathcal{T}|u_n^{\mathrm{I}}(k)\rangle & \langle u_n^{\mathrm{I}}(-k)|\mathcal{T}|u_n^{\mathrm{II}}(k)\rangle\\ \langle u_n^{\mathrm{II}}(-k)|\mathcal{T}|u_n^{\mathrm{I}}(k)\rangle & \langle u_n^{\mathrm{II}}(-k)|\mathcal{T}|u_n^{\mathrm{II}}(k)\rangle\end{pmatrix}\\ &= \sum_n 1_{n,n}\otimes\begin{pmatrix}e^{-\mathrm{i}\chi_n(-k)}\langle u_n^{\mathrm{I}}(-k)|u_n^{\mathrm{II}}(-k)\rangle & -e^{-\mathrm{i}\chi_n(k)}\langle u_n^{\mathrm{I}}(-k)|u_n^{\mathrm{I}}(-k)\rangle\\ e^{-\mathrm{i}\chi_n(-k)}\langle u_n^{\mathrm{II}}(-k)|u_n^{\mathrm{II}}(-k)\rangle & -e^{-\mathrm{i}\chi_n(k)}\langle u_n^{\mathrm{II}}(-k)|u_n^{\mathrm{I}}(-k)\rangle\end{pmatrix}\\ &= \sum_n 1_{n,n}\otimes\begin{pmatrix}0 & -e^{-\mathrm{i}\chi_n(k)}\\ e^{-\mathrm{i}\chi_n(-k)} & 0\end{pmatrix}, \end{aligned} \tag{12}$$

where $1_{n,n}$ is an $N\times N$ matrix whose elements are 1 for (n,n) and 0 otherwise[*5]. Thus, w satisfies

$$w^T(k) = -w(-k). \tag{13}$$

Specifically, at a time-reversal-invariant momentum $k = k_{\mathrm{TRIM}} \in \{0,\pi\}$, w becomes an antisymmetric matrix, and we have

$$\mathrm{Pf}\; w(k_{\mathrm{TRIM}}) = \prod_n\left(-e^{-\mathrm{i}\chi_n(k_{\mathrm{TRIM}})}\right) = (-1)^N e^{-\mathrm{i}\sum_n\chi_n(k_{\mathrm{TRIM}})}. \tag{14}$$

[*4] The gauge transformation

$$|u_n(k)\rangle \mapsto \sum_m U_{nm}(k)|u_m(k)\rangle \tag{6}$$

leads to

$$w(k) \mapsto U^*(-k)\, w(k)\, U^\dagger(k), \tag{7}$$
$$\mathrm{Pf}\, w(k_{\mathrm{TRIM}}) \mapsto (\mathrm{Pf}\, w(k_{\mathrm{TRIM}}))(\det U^*(k_{\mathrm{TRIM}})). \tag{8}$$

[*5] While the matrix elements of w seem different from those in Ref. [1], the final formula is identical.

Thus, Eq. (11) reduces to

$$P^{\mathrm{I}} = \frac{1}{2\pi} \left[\int_0^{\pi} dk\, A\left(k\right) - \mathrm{i} \log \left(\frac{\mathrm{Pf}\ w\left(\pi\right)}{\mathrm{Pf}\ w\left(0\right)} \right) \right]. \tag{15}$$

Similarly, we have

$$P^{\mathrm{II}} = \frac{1}{2\pi} \left[\int_0^{\pi} dk\, A\left(-k\right) + \mathrm{i} \log \left(\frac{\mathrm{Pf}\ w\left(\pi\right)}{\mathrm{Pf}\ w\left(0\right)} \right) \right], \tag{16}$$

leading to

$$P_{\theta} \coloneqq P^{\mathrm{I}} - P^{\mathrm{II}} = \frac{1}{2\pi} \left[\int_0^{\pi} dk \left(A\left(k\right) - A\left(-k\right) \right) - 2\mathrm{i} \log \left(\frac{\mathrm{Pf}\ w\left(\pi\right)}{\mathrm{Pf}\ w\left(0\right)} \right) \right]. \tag{17}$$

Here, we notice

$$\begin{aligned}
\mathrm{i}\, \mathrm{tr} \left(w^{\dagger}\left(k\right) \partial_k w\left(k\right) \right) &= \mathrm{i} \sum_{mn} w_{nm}^{*} \partial_k w_{nm}\left(k\right) \\
&= \mathrm{i} \sum_{mn} \langle u_m\left(k\right) | T^{\dagger} | u_n\left(-k\right) \rangle\, \partial_k \langle u_n\left(-k\right) | T | u_m\left(k\right) \rangle \\
&= \mathrm{i} \sum_{n} \left[\langle u_n\left(k\right) | \partial_k u_n\left(k\right) \rangle + \langle \partial_k u_n\left(-k\right) | u_n\left(-k\right) \rangle \right] \\
&= A\left(k\right) - A\left(-k\right),
\end{aligned} \tag{18}$$

and thus have

$$\begin{aligned}
P_{\theta} &= -\frac{1}{2\pi\mathrm{i}} \left[\int_0^{\pi} dk\, \mathrm{tr} \left(w^{\dagger}\left(k\right) \partial_k w\left(k\right) \right) - 2 \log \left(\frac{\mathrm{Pf}\ w\left(\pi\right)}{\mathrm{Pf}\ w\left(0\right)} \right) \right] \\
&= -\frac{1}{2\pi\mathrm{i}} \left[\int_0^{\pi} dk\, \partial_k \log \det \left(w\left(k\right) \right) - 2 \log \left(\frac{\mathrm{Pf}\ w\left(\pi\right)}{\mathrm{Pf}\ w\left(0\right)} \right) \right] \\
&= -\frac{1}{\pi\mathrm{i}} \log \left[\frac{\mathrm{Pf}\, w\left(0\right)}{\sqrt{\det w\left(0\right)}} \frac{\mathrm{Pf}\, w\left(\pi\right)}{\sqrt{\det w\left(\pi\right)}} \right].
\end{aligned} \tag{19}$$

Notably, since $\det w$ is a complex function, its square root $\sqrt{\det w}$ has two branches. Here, we have to appropriately choose $\sqrt{\det w}$ such that the branch at $k=0$ is continuously connected to that at $k=\pi$. Given the relation $\det w = \left(\mathrm{Pf}\, w\right)^2$, we have $\left(\mathrm{Pf}\, w\right) / \sqrt{\det w} = \pm 1$, leading to $P_{\theta} \in \mathbb{Z}$ and Eq. (5). The ambiguity of the logarithm means that $P_{\theta} \in \mathbb{Z}$ is well defined modulo 2.

In the additional presence of chiral symmetry that anticommutes with time-reversal symmetry (i.e., class DIII), the time-reversal polarization P_{θ} (mod 2) gives a $\mathbb{Z}_2$ topological invariant (see, for example, Refs. [3,4] for further details).

2 $\mathbb{Z}_2$ topological invariant

Now, we consider a two-dimensional band insulator $H(k_x, k_y)$ that respects time-reversal symmetry in Eq. (1) and introduce the Fu-Kane $\mathbb{Z}_2$ topological invariant as a pump of the time-reversal polarization. At each time-reversal-invariant momentum $k_y = k_{\mathrm{TRIM}} \in \{0, \pi\}$ along the y direction, the Hamiltonian $H(k_x, k_y = k_{\mathrm{TRIM}})$ can be regarded as a time-reversal-invariant one-dimensional band insulator along the x direction. Consequently, we can introduce the time-reversal polarization $P_\theta(k_y = k_{\mathrm{TRIM}})$. While $P_\theta(k_y = k_{\mathrm{TRIM}})$ itself is gauge dependent, the continuous change (pump) from $k_y = 0$ to $k_y = \pi$ gives a gauge-invariant $\mathbb{Z}_2$ topological invariant

$$\nu := P_\theta(k_y = \pi) - P_\theta(k_y = 0) \pmod 2 . \tag{20}$$

Moreover, from Eq. (5), this $\mathbb{Z}_2$ topological invariant can be expressed as

$$(-1)^\nu = \prod_{i=1}^{4} \frac{\mathrm{Pf}\, w(\Gamma_i)}{\sqrt{\det w(\Gamma_i)}} \tag{21}$$

with time-reversal-invariant momenta $\Gamma_i \in \{(0,0), (0,\pi), (\pi,0), (\pi,\pi)\}$ ($i = 1,2,3,4$) in the two-dimensional Brillouin zone. Notably, to apply this formula, wave functions should be defined continuously over the entire two-dimensional Brillouin zone. This is always possible since time-reversal symmetry enforces the vanishing of the Chern number.

References

[1] L. Fu and C. L. Kane, *Time reversal polarization and a Z_2 adiabatic spin pump*, Phys. Rev. B **74**, 195312 (2006) [arXiv:cond-mat/0606336].

[2] C. L. Kane and E. J. Mele, *Z_2 Topological Order and the Quantum Spin Hall Effect*, Phys. Rev. Lett. **95**, 146802 (2005) [arXiv:cond-mat/0506581].

[3] X.-L. Qi, T. L. Hughes, and S.-C. Zhang, *Topological invariants for the Fermi surface of a time-reversal-invariant superconductor*, Phys. Rev. B **81**, 134508 (2010) [arXiv:0908.3550].

[4] A. P. Schnyder and S. Ryu, *Topological phases and surface flat bands in superconductors without inversion symmetry*, Phys. Rev. B **84**, 060504(R) (2011) [arXiv:1011.1438].