PT Symmetry and Topological Invariants (Draft)

Ken Shiozaki

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Abstract

PT symmetry satisfying $(PT)^2 = 1$ contains many technical topics in topological insulators protected by crystalline symmetry: topological invariants beyond irreducible representations, the relation between topological invariants as transition functions and Berry phases, the relation between localization positions of degrees of freedom and topological invariants, fragile topological insulators, and examples of topological invariants that do not behave additively under direct sums of bands. As a reference, see the appendix of [1].

1 PT symmetry

Use a basis that is periodic in the BZ. Let d be the spatial dimension. The PT symmetry is

$$V_{\boldsymbol{k}} H^*_{\boldsymbol{k}} V_{\boldsymbol{k}} = H_{\boldsymbol{k}}, \quad V_{\boldsymbol{k}} V^*_{\boldsymbol{k}} = 1. \tag{1}$$

We want to classify vector bundles that can arise as the occupied states of the Hamiltonian $H_{\boldsymbol{k}}$. The unitary matrix $V_{\boldsymbol{k}}$ is determined by the localization positions of the degrees of freedom. Both the Hamiltonian $H_{\boldsymbol{k}}$ and the PT-symmetry matrix $U_{\boldsymbol{k}}$ are globally defined on the BZ. For example, when a degree of freedom is located at an inversion-symmetric point $\boldsymbol{x} = \boldsymbol{n}/2$, $\boldsymbol{n} \in \mathbb{Z}^d$, inside a unit cell, the 1×1 matrix is

$$V_{\boldsymbol{k}} = z e^{i\boldsymbol{k}\cdot\boldsymbol{n}}, \tag{2}$$

where z is a $U(1)$ phase. When degrees of freedom occur in an inversion-symmetric pair $\boldsymbol{x}, -\boldsymbol{x}$, where $\boldsymbol{x}$ is the displacement vector from the center of the unit cell, the matrix is the 2×2 matrix

$$V_{\boldsymbol{k}} = \begin{pmatrix} & z \\ z^* & \end{pmatrix}. \tag{3}$$

In general, $V_{\boldsymbol{k}}$ is complex symmetric, $V^T_{\boldsymbol{k}} = V_{\boldsymbol{k}}$, and therefore by general theory, using a basis $Q_{\boldsymbol{k}} = (|u^1_{\boldsymbol{k}}\rangle, \dots, |u^N_{\boldsymbol{k}}\rangle)$, one can write

$$V_{\boldsymbol{k}} Q^*_{\boldsymbol{k}} = Q_{\boldsymbol{k}} \begin{pmatrix} e^{i\theta^1_{\boldsymbol{k}}} & & \\ & \ddots & \\ & & e^{i\theta^N_{\boldsymbol{k}}} \end{pmatrix}. \tag{4}$$

- Can $Q_{\boldsymbol{k}}$ be chosen globally?

Let $H_{\boldsymbol{k}}$ be an $N \times N$ matrix. Choose a good cover $\{U_i\}$ of the BZ. On a patch U_i, the set of bases $\Phi^i_{\boldsymbol{k}}$ of the occupied states of the Hamiltonian $H_{\boldsymbol{k}}$ can be chosen to satisfy the PT-symmetric gauge condition

$$V_{\boldsymbol{k}} (\Phi^i_{\boldsymbol{k}})^* = \Phi^i_{\boldsymbol{k}}. \tag{5}$$

Note that the PT-symmetry matrix $V_{\boldsymbol{k}}$ is globally defined. Let n be the number of occupied states. Then $\Phi^i_{\boldsymbol{k}}$ is a quasi-unitary $N \times n$ matrix satisfying $(\Phi^i_{\boldsymbol{k}})^\dagger \Phi^i_{\boldsymbol{k}} = 1_n$. On the overlap $U_{ij} = U_i \cap U_j$, the transition function

$$t^{ij}_{\boldsymbol{k}} = (\Phi^i_{\boldsymbol{k}})^\dagger \Phi^j_{\boldsymbol{k}}, \quad \boldsymbol{k} \in U_{ij}, \tag{6}$$

is defined. The matrix $t^{ij}_{\boldsymbol{k}}$ is real. Indeed, using

$$(\Phi^i_{\boldsymbol{k}})^* = V^\dagger_{\boldsymbol{k}} \Phi^i_{\boldsymbol{k}}, \tag{7}$$

one obtains

$$(t^{ij}_{\boldsymbol{k}})^* = (\Phi^i_{\boldsymbol{k}})^\dagger V_{\boldsymbol{k}} V^\dagger_{\boldsymbol{k}} \Phi^j_{\boldsymbol{k}} = (\Phi^i_{\boldsymbol{k}})^\dagger \Phi^j_{\boldsymbol{k}} = t^{ij}_{\boldsymbol{k}}. \tag{8}$$

The classification of homotopy classes of the transition functions $t^{ij}_{\boldsymbol{k}}$ taking values in $O(n)$ gives the classification of PT-symmetric insulators.

By definition, topological invariants are given by the classification of $t^{ij}_{\boldsymbol{k}}$. However, because this imposes conditions that are inconvenient for numerical calculations, such as the construction of smooth bases $\Phi^i_{\boldsymbol{k}}$ and a PT-symmetric gauge, one often rewrites the invariant in a relaxed form that is easier to compute numerically.

2 One-dimensional systems

First consider a one-dimensional system. One may take a single patch $[0, 2\pi]$, and assume that it satisfies the PT-symmetric gauge condition

$$V_k \Phi^*_k = \Phi_k. \tag{9}$$

The transition function at $k = 0 = 2\pi$ is

$$t = \Phi^\dagger_0 \Phi_{2\pi} \in O(n). \tag{10}$$

It is classified by the $\mathbb{Z}_2$ value

$$\det t \in \pm 1, \tag{11}$$

and $\det t$ is the topological invariant. Indeed, under a PT-symmetric gauge transformation

$$\Phi_k \mapsto \Phi_k W_k, \quad W_k \in O(n), \tag{12}$$

where W_k is continuous on $[0, 2\pi]$ and $W_{2\pi}$ need not be equal to W_0, one has

$$t \mapsto W^T_0 t W_{2\pi}. \tag{13}$$

Since $\det W_k$ is constant, $\det t$ is gauge invariant.

Let us look for an expression for the topological invariant t that removes the PT-symmetric gauge condition. Under a general gauge transformation without imposing the PT gauge,

$$\Phi_k \mapsto \Phi_k W_k, \quad W_k \in U(n), \tag{14}$$

we have

$$\det t \mapsto \det W^\dagger_0 \det t \det W_{2\pi}, \tag{15}$$

so $\det t$ changes under the gauge transformation. To make it gauge invariant, add a Berry-phase term. The following $U(1)$ value is gauge invariant:

$$e^{i\gamma} = \det(\Phi^\dagger_0 \Phi_{2\pi}) e^{-\int_0^{2\pi} \mathrm{tr}\, \Phi^\dagger_k d\Phi_k} \in U(1). \tag{16}$$

Let us examine whether this quantity agrees with t. Since Φ_k is uniquely defined on $[0, 2\pi]$, note that there is no $2\pi i\mathbb{Z}$ ambiguity in $\int_0^{2\pi} \mathrm{tr}\, \Phi^\dagger_k d\Phi_k$. Impose the PT-symmetric gauge

$$\Phi^*_k = V^*_k \Phi_k. \tag{17}$$

[1] Using $(\mathrm{tr}\,\Phi^\dagger d\Phi)^* = -\mathrm{tr}\,\Phi^\dagger d\Phi$, we get

$$-\int_0^{2\pi} \mathrm{tr}\,\Phi_k^\dagger d\Phi_k = \int_0^{2\pi} \mathrm{tr}\,(\Phi_k^\dagger d\Phi_k)^* \tag{18}$$

$$= \int_0^{2\pi} \mathrm{tr}\,\Phi_k^\dagger V_k^T d(V_k^* \Phi_k) \tag{19}$$

$$= \int_0^{2\pi} \mathrm{tr}\,\Phi_k^\dagger d\Phi_k + \int_0^{2\pi} \mathrm{tr}\,\Phi_k^\dagger (V_k^T dV_k^*)\Phi_k. \tag{20}$$

Therefore

$$-\int_0^{2\pi} \mathrm{tr}\,\Phi_k^\dagger d\Phi_k = \frac{1}{2}\int_0^{2\pi} \mathrm{tr}\,\Phi_k^\dagger (V_k^T dV_k^*)\Phi_k. \tag{21}$$

Note that the right-hand side is gauge invariant. When the PT-symmetric gauge is imposed,

$$e^{i\gamma} = \det(\Phi_0^\dagger \Phi_{2\pi}) e^{\frac{1}{2}\int_0^{2\pi} \mathrm{tr}\,\Phi_k^\dagger (V_k^T dV_k^*)\Phi_k} = \det t \times e^{\frac{1}{2}\int_0^{2\pi} \mathrm{tr}\,\Phi_k^\dagger (V_k^T dV_k^*)\Phi_k}. \tag{22}$$

Thus one obtains an expression for the $\mathbb{Z}_2$ invariant without imposing the PT-symmetric gauge condition:

$$\boxed{\det t = e^{i\gamma} e^{-i\beta}, \quad e^{i\beta} := e^{\frac{1}{2}\int_0^{2\pi} \mathrm{tr}\,\Phi_k^\dagger (V_k^T dV_k^*)\Phi_k}.} \tag{23}$$

Here the first factor $e^{i\gamma}$ is the Berry phase and is gauge invariant. The second factor $e^{i\beta}$ is also gauge invariant, since it does not change under the gauge transformation $\Phi_k \mapsto \Phi_k W_k$.

- Are $e^{i\gamma}$ and $e^{i\beta}$ individually $\mathbb{Z}_2$-valued? Or is only the combination $\mathbb{Z}_2$-valued?

2.1 Examples

- If $V_k = 1$ and $\Phi_k \sim (1)$, then

$$e^{i\gamma} = 1, \quad e^{i\beta} = 1, \tag{24}$$

  and hence

$$\det t = 1. \tag{25}$$

- If $V_k = e^{ik}$ and $\Phi_k \sim (1)$, then

$$e^{i\gamma} = 1, \quad e^{i\beta} = -1, \tag{26}$$

  and hence

$$\det t = -1. \tag{27}$$

- If $V_k = 1_2$ and $\Phi_k \sim (\cos\frac{k}{2}, \sin\frac{k}{2})^T$, then

$$e^{i\gamma} = -1, \quad e^{i\beta} = 1, \tag{28}$$

  and hence

$$\det t = -1. \tag{29}$$

- If $V_k = e^{ik} 1_2$ and $\Phi_k \sim (\cos\frac{k}{2}, \sin\frac{k}{2})^T$, then

$$e^{i\gamma} = -1, \quad e^{i\beta} = -1, \tag{30}$$

  and hence

$$\det t = 1. \tag{31}$$

These are some examples. Note that the result agrees with the localization position of the Wannier state constructed from the occupied state.

[1] This seems to have better properties than $\Phi_k^* = V_k^\dagger \Phi_k$.

2.2 A basis that is nonperiodic in the BZ

Consider the Fourier transform from real space to momentum space

$$|k,a\rangle' = \sum_R |R+x_a\rangle\, e^{ik(R+x_a)}, \tag{32}$$

where the displacement x_a of the degree of freedom from the unit-cell center R is included in the basis. Since

$$|k,a\rangle' = |k+2\pi,b\rangle'\, U_{ba}(2\pi), \quad U_{ba}(k) = \delta_{ba} e^{-ikx_b}, \tag{33}$$

the Hamiltonian satisfies the boundary condition

$$U(2\pi)H(k)U(2\pi)^\dagger = H(k+2\pi). \tag{34}$$

Its relation to the Hamiltonian H_k that is periodic in the BZ is

$$H_k = U(k)^\dagger H(k) U(k). \tag{35}$$

For the occupied states and the matrix of PT symmetry, respectively, we also have

$$\Phi_k = U(k)^\dagger \Phi(k), \tag{36}$$

$$V_k = U(k)^\dagger V(k) U(k)^*. \tag{37}$$

Rewrite the expression for the $\mathbb{Z}_2$ invariant in a basis that is nonperiodic in the BZ. The Berry phase is

$$\begin{aligned} e^{i\gamma} &= \det(\Phi_0^\dagger \Phi_{2\pi}) \exp\left[-\int_0^{2\pi} \mathrm{tr}\, \Phi_k^\dagger d\Phi_k\right] && (38)\\ &= \det[\Phi(0)^\dagger U(0) U(2\pi)^\dagger \Phi(2\pi)] \exp\left[-\int_0^{2\pi} \mathrm{tr}\, \Phi(k)^\dagger U(k) d\{U(k)^\dagger \Phi(k)\}\right] && (39)\\ &= \det[\Phi(0)^\dagger U(2\pi)^\dagger \Phi(2\pi)] \exp\left[-\int_0^{2\pi} \mathrm{tr}\, \Phi(k)^\dagger d\Phi(k)\right] \exp\left[-\int_0^{2\pi} \mathrm{tr}\, \Phi(k)^\dagger U(k) dU(k)^\dagger \Phi(k)\right]. && (40) \end{aligned}$$

Thus it is the product of the Berry phase in the nonperiodic basis,

$$e^{i\gamma_{\rm NP}} = \det[\Phi(0)^\dagger U(2\pi)^\dagger \Phi(2\pi)] \exp\left[-\int_0^{2\pi} \mathrm{tr}\, \Phi(k)^\dagger d\Phi(k)\right], \tag{41}$$

and the correction term

$$e^{-i\delta} := \exp\left[-\int_0^{2\pi} \mathrm{tr}\, \Phi(k)^\dagger U(k) dU(k)^\dagger \Phi(k)\right]. \tag{42}$$

For $e^{i\beta}$, one has

$$\begin{aligned} e^{i\beta} &= \exp\left[\frac{1}{2}\int_0^{2\pi} \mathrm{tr}\, \Phi_k^\dagger (V_k^T dV_k^*) \Phi_k\right] && (43)\\ &= \exp\left[\frac{1}{2}\int_0^{2\pi} \mathrm{tr}\, \Phi(k)^\dagger U(k) (U(k)^\dagger V(k) U(k)^*)^T d(U(k)^\dagger V(k) U(k)^*)^* U(k)^\dagger \Phi(k)\right] && (44)\\ &= \exp\left[\frac{1}{2}\int_0^{2\pi} \mathrm{tr}\, \Phi(k)^\dagger \{V(k)^T U(k)^* dU(k)^T V(k)^* + V(k)^T dV(k)^* + dU(k) U(k)^\dagger\} \Phi(k)\right]. && (45) \end{aligned}$$

Since $\Phi(k)$ satisfies PT symmetry, there exists a unitary matrix $w(k)$ such that

$$V(k)\Phi(k)^* = \Phi(k) w(k). \tag{46}$$

Therefore the first term gives

$$\exp\left[\frac{1}{2}\int_0^{2\pi}\operatorname{tr} w(k)^T\Phi(k)^T U(k)^* dU(k)^T\Phi(k)^* w(k)^*\right] \tag{47}$$

$$= \exp\left[\frac{1}{2}\int_0^{2\pi}\operatorname{tr}\Phi(k)^T U(k)^* dU(k)^T\Phi(k)^*\right] \tag{48}$$

$$= \exp\left[\frac{1}{2}\int_0^{2\pi}\operatorname{tr}\Phi(k)^\dagger dU(k)U(k)^\dagger\Phi(k)\right]. \tag{49}$$

It follows that

$$e^{i\beta} = \exp\left[\frac{1}{2}\int_0^{2\pi}\operatorname{tr}\Phi(k)^\dagger\{V(k)^T dV(k)^* + 2dU(k)U(k)^\dagger\}\Phi(k)\right] \tag{50}$$

$$= \exp\left[\frac{1}{2}\int_0^{2\pi}\operatorname{tr}\Phi(k)^\dagger\{V(k)^T dV(k)^* - 2U(k)dU(k)^\dagger\}\Phi(k)\right] \tag{51}$$

$$= \exp\left[\frac{1}{2}\int_0^{2\pi}\operatorname{tr}\Phi(k)^\dagger V(k)^T dV(k)^*\Phi(k)\right]e^{-i\delta}. \tag{52}$$

Therefore

$$e^{i\beta}e^{i\delta} = \exp\left[\frac{1}{2}\int_0^{2\pi}\operatorname{tr}\Phi(k)^\dagger V(k)^T dV(k)^*\Phi(k)\right]. \tag{53}$$

Thus the expression for the $\mathbb{Z}_2$ invariant in the nonperiodic basis is

$$\det t = e^{i\gamma_{\mathrm{NP}}}e^{-i\beta_{\mathrm{NP}}}, \quad e^{i\beta_{\mathrm{NP}}} = \exp\left[\frac{1}{2}\int_0^{2\pi}\operatorname{tr}\Phi(k)^\dagger V(k)^T dV(k)^*\Phi(k)\right]. \tag{54}$$

Note that this is completely equal to the expression for the $\mathbb{Z}_2$ invariant in the periodic basis. In fact, $e^{i\beta_{\mathrm{NP}}}$ is determined only by the definition of PT symmetry and the number of occupied states; it does not depend on the details of the occupied states. In the nonperiodic basis, if the real-space action of the PT transformation is $PT : x \mapsto -x + 2a_{\mathrm{PT}}$, where a_{PT} is the inversion center, then using a k-independent unitary matrix D, one has

$$V(k) := e^{-ik2a_{\mathrm{PT}}}D. \tag{55}$$

Thus, if ν is the number of occupied states, or the number of electrons per unit cell,

$$e^{i\beta_{\mathrm{NP}}} = e^{2\pi i\nu a_{\mathrm{PT}}}. \tag{56}$$

In the end, we have shown that

$$\det t = e^{i\gamma}e^{-i\beta} = e^{i\gamma_{NP}}e^{-i\delta} = e^{i\gamma_{NP}}e^{-2\pi i\nu a_{\mathrm{PT}}}. \tag{57}$$

Furthermore, recalling that the Berry phase $e^{i\gamma_{NP}}$ in the nonperiodic basis is the localization position, or sum of localization positions, of the Wannier states,

$$\frac{\gamma_{NP}}{2\pi} = \sum_{n=1}^{\nu}\langle W_{nR}\,|\,\hat{r} - R\,|\,W_{nR}\rangle = \langle\hat{r}\rangle \in \mathbb{R}/\mathbb{Z}, \tag{58}$$

we obtain

$$\det t = e^{2\pi i(\langle\hat{r}\rangle - \nu a_{\mathrm{PT}})}. \tag{59}$$

In particular, for one band, $\nu = 1$,

$$\det t = e^{2\pi i(\langle\hat{r}\rangle - a_{\mathrm{PT}})}. \tag{60}$$

Thus the $\mathbb{Z}_2$ invariant $\det t$ has the physical meaning of the displacement of the occupied state from the inversion center.

2.3 Dependence on the choice of unit-cell center

The $\mathbb{Z}_2$ invariant does not depend on the choice of the center position of the unit cell. This is clear because changing the choice of the unit-cell center is a continuous change, but it can also be checked from the expression for the invariant. Under a change of the choice of the unit-cell center

$$R \mapsto R + \delta R, \tag{61}$$

the localization position of the occupied states changes as

$$\langle \hat{r} \rangle \mapsto \langle \hat{r} \rangle + \nu \delta R. \tag{62}$$

On the other hand, the inversion center changes as

$$a_{\mathrm{PT}} \mapsto a_{\mathrm{PT}} + \delta R. \tag{63}$$

Thus the contributions cancel, and the $\mathbb{Z}_2$ invariant $\det t$ is unchanged.

2.4 Dependence on the choice of inversion center

On the other hand, the $\mathbb{Z}_2$ invariant depends on the choice of inversion center. There is an ambiguity in the choice of inversion center. This is the freedom of a gauge transformation of a section from the point group to the space group. That is, for an arbitrary integer $n \in \mathbb{Z}$, one may choose

$$\{PT|n + 2a_{\mathrm{PT}}\} = \{1|n\}\{PT|2a_{\mathrm{PT}}\} : x \mapsto -x + 2a_{\mathrm{PT}} + n \tag{64}$$

as the spatial inversion. Under this transformation, the inversion center changes as

$$a_{\mathrm{PT}} \mapsto a_{\mathrm{PT}} + \frac{n}{2}. \tag{65}$$

In the expression

$$\det t = e^{2\pi i (\langle \hat{r} \rangle - \nu a_{\mathrm{PT}})}, \tag{66}$$

the expectation value of the localization position, $\langle \hat{r} \rangle$, is defined independently of the PT transformation, so it does not depend on the choice of a_{PT}. Therefore

$$\det t = e^{2\pi i (\langle \hat{r} \rangle - \nu a_{\mathrm{PT}})} \mapsto e^{2\pi i (\langle \hat{r} \rangle - \nu (a_{\mathrm{PT}} + \frac{n}{2}))} = \det t \times e^{-\pi i \nu n}. \tag{67}$$

Consequently, when the number of occupied bands ν is even, the $\mathbb{Z}_2$ invariant $\det t$ does not depend on the choice of inversion center.

3 Two dimensions

- The second Stiefel–Whitney class and direct sums of bands.
- Fragile topology.

References

[1] Junyeong Ahn, Dongwook Kim, Youngkuk Kim, Bohm-Jung Yang, *Band Topology and Linking Structure of Nodal Line Semimetals with Z2 Monopole Charges*, arXiv:1803.11416.