Classification of "Real" Bloch-bundles: topological insulators of type AI

Giuseppe De Nittis

(*FAU, Universität Erlangen-Nürnberg*)

EPSRC Symposium: Many-Body Quantum Systems

University of Warwick, U.K.   17-21 March, 2014

Joint work with:

K. Gomi

Reference:

arXiv:1402.1284

FRIEDRICH-ALEXANDER UNIVERSITÄT ERLANGEN-NÜRNBERG

Alexander von Humboldt Stiftung/Foundation

Outline

Band Insulators

- For an enlightened explanation about the physical point of view the main reference is

  !! Graf's talk of last Tuesday 18th !!

  I will focus only on the mathematical (topological) aspects.

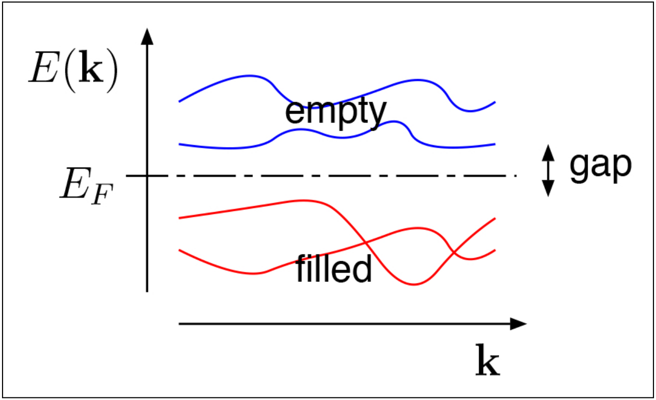
- The Bloch-Floquet theory exploits the translational symmetry of a crystal structure to describe electronic states in terms of their crystal momentum k, defined in a periodic Brillouin zone $\mathbb{B}$.

- A little bit more in general one can assume that:

  "*the electronic properties of a crystal are described by a family of Hamiltonians labelled by points of a manifold* $\mathbb{B}$"

$$\mathbb{B} \ni k \longmapsto H(k) \,.$$

In a band insulator an energy gap separates the filled valence bands from the empty conduction bands. The Fermi level E_F characterizes the gap.



The energy bands $E(k)$ are the eigenvalues of $H(k)$

$$H(k)\,\psi(k) = E(k)\,\psi(k) \qquad k \in \mathbb{B}\,.$$

A rigorous classification scheme requires (in my opinion !!) three ingredients:

«A» The interpretation of the "vague" notion of topological insulator in terms of a mathematical structure (category) for which the notion of classification makes sense (objects, isomorphisms, equivalence classes, ...).

«B» A classification theorem.

«C» An (hopefully !!) algorithmic method to compute the classification and a set of proper labels to discern between different (non-isomorphic) objects.

Bloch Bundle and Vector Bundle Theory

For all $k \in \mathbb{B}$ the operator $H(k)$ is a self-adjoint $N \times N$ matrix with real eigenvalues

$$E_1(k) \leqslant E_2(k) \leqslant \ldots \leqslant E_{N-1}(k) \leqslant E_N(k)$$

and related eigenvectors $\psi_j(k)$, $j = 1, \ldots, N$.

Definition (Gap condition)

There exists a $E_F \in \mathbb{R}$ and an integer $1 < M < N$ such that:

$$\begin{cases} E_M(k) < E_F \\ E_{M+1}(k) > E_F \end{cases} \qquad \forall k \in \mathbb{B} \,.$$

The Fermi projection onto the filled states is the matrix-valued map $\mathbb{B} \ni k \mapsto P_F(k)$ defined by

$$P_F(k) := \sum_{j=1}^{M} |\psi_j(k)\rangle\langle\psi_j(k)| \,.$$

- For each $k \in \mathbb{B}$

$$\mathscr{H}_k := \mathrm{Ran}\, P_F(k) \subset \mathscr{H}$$

  is a subspace of $\mathbb{C}^N$ of dimension M.

- The collection

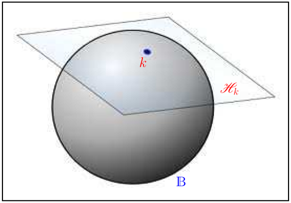
$$\mathscr{E}_F := \bigsqcup_{k \in \mathbb{B}} \mathscr{H}_k$$

  is a topological space (said total space) and the map

$$\pi : \mathscr{E}_F \longrightarrow \mathbb{B}$$

  defined by $\pi(k, \mathrm{v}) = k$ is continuous (and open).

- $\pi : \mathscr{E}_F \to \mathbb{B}$ is a complex vector bundle called Bloch bundle.



Gapped band insulator (of type A) at Fermi energy E_F

$\Updownarrow$

Rank M complex vector bundle over $\mathbb{B}$

$\Updownarrow$ (homotopy **classification theorem**)

$$\mathrm{Vec}^M_{\mathbb{C}}(\mathbb{B}) \simeq [\mathbb{B}, \mathrm{Gr}_M(\mathbb{C}^N)] \qquad (N \gg 1)$$

The space

$$\mathrm{Gr}_M(\mathbb{C}^N) := \mathbb{U}(N) \,/\, \big(\mathbb{U}(M) \times \mathbb{U}(N-M)\big) \,.$$

is the Grasmannian of M-planes in $\mathbb{C}^N$.

☞ **Remark:** The computation of $[\mathbb{B}, \mathrm{Gr}_M(\mathbb{C}^N)]$ is, generally, an extremely difficult task (non algorithmic problem **!!**). Explicit computations are available only for simple spaces $\mathbb{B}$.

The Case of Free Fermions: $\mathbb{B} \equiv \mathbb{S}^d$

For a system of free fermions (after a Fourier transform)

$$\mathbb{S}^d := \{k \in \mathbb{R}^{d+1} \mid \|k\| = 1\} \simeq \mathbb{R}^d \cup \{\infty\} .$$

Number of different phases of a band insulator of type A

$$\Updownarrow$$

$$\pi_d(\mathrm{Gr}_M(\mathbb{C}^N)) := [\mathbb{S}^d, \mathrm{Gr}_M(\mathbb{C}^N)]$$

$\pi_d(X)$ is the d-th homotopy group of the space X.

✧ **Problem:** How to compute the homotopy of $\mathrm{Gr}_M(\mathbb{C}^N)$?

Theorem (Bott, 1959)

$$\pi_d(\mathrm{Gr}_M(\mathbb{C}^N)) = \pi_{d-1}(\mathbb{U}(M)) \qquad \textit{if} \qquad 2N \geqslant 2M + d + 1 .$$

Homotopy groups of $\mathbb{U}(M)$

$\pi_d(\mathbb{U}(M))$	$d=0$	$d=1$	$d=2$	$d=3$	$d=4$	$d=5$
M=1	0	$\mathbb{Z}$	0	0	0	0
M=2	0	$\mathbb{Z}$	0	$\mathbb{Z}$	$\mathbb{Z}_2$	$\mathbb{Z}_2$
M=3	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$
M=4	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$
M=5	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$

The stable regime is defined by $d < 2M$ (in blu the values for the unstable case). In the stable regime one has the Bott periodicity

$$\pi_d(\mathbb{U}(M)) = \begin{cases} 0 & \text{if} \quad d \ \text{even} \quad \text{or} \quad d=0 \\ \mathbb{Z} & \text{if} \quad d \ \text{odd} \\ \mathbb{Z}_{M!} & \text{if} \quad d = 2M \, . \end{cases} \qquad (d \leqslant 2M)$$

Topological Insulators in class A ($\mathbb{B} = \mathbb{S}^d$)

The number of topological phases depends on the dimension d and on the number of filled states M (this is missed in K-theory **!!**)

$d=1$	$d=2$	$d=3$	$d=4$	$d=5$	...
0	$\mathbb{Z}$	0	$0 \quad (M=1)$ $\mathbb{Z} \quad (M \geqslant 2)$	$0 \quad (M=1)$ $\mathbb{Z}_2 \quad (M=2)$ $0 \quad (M \geqslant 3)$	...

$d=1$ Band insulators show only the trivial phase (ordinary insulators).

$d=2$ For every integer there exists a topological phase and band insulators in different phases cannot be deformed into each other without "altering the nature" of the system (*e.g.* quantum Hall insulators).

$d=3$ As in the case $d=1$.

$d=4$ A difference between the non-stable case $M=1$ and the stable case $M \geqslant 2$ appears. The value of M is dictated by physics **!!**

Ordinary insulator:

Band insulator in a trivial phase

$\Updownarrow$

Trivial vector bundle

$\Updownarrow$

Exists a global frame of continuous Bloch functions

Allowed (adiabatic) deformations:

Transformations which doesn't alter the nature of the system

$\Updownarrow$

Stability of the topological phase

$\Updownarrow$

Vector bundle isomorphism

The Case of Bloch Electrons: $\mathbb{B} \equiv \mathbb{T}^d$

Electrons interacting with the crystalline structure of a metal (Bloch-Floquet)

$$\mathbb{B} = \mathbb{T}^d := \mathbb{S}^1 \times \ldots \times \mathbb{S}^1 \qquad (d\text{-times}) .$$

The computation of $[\mathbb{T}^d, \mathrm{Gr}_M(\mathbb{C}^N)]$ is non trivial. The theory of characteristic class becomes relevant (since algorithmic !!).

Theorem (Peterson, 1959)

If $\dim(X) \leqslant 4$ *then*

$$\mathrm{Vec}^1_{\mathbb{C}}(X) \simeq H^2(X,\mathbb{Z})$$
$$\mathrm{Vec}^M_{\mathbb{C}}(X) \simeq H^2(X,\mathbb{Z}) \oplus H^4(X,\mathbb{Z}) \qquad (M \geqslant 2)$$

and the isomorphism

$$\mathrm{Vec}^M_{\mathbb{C}}(X) \ni [\mathscr{E}] \longmapsto (c_1, c_2) \in H^2(X,\mathbb{Z}) \oplus H^4(X,\mathbb{Z})$$

is given by the first two Chern classes ($c_2 = 0$ if $M = 1$).

	$d=1$	$d=2$	$d=3$	$d=4$
$\mathbb{B}=\mathbb{S}^d$	0	$\mathbb{Z}$	0	0 $(M=1)$ $\mathbb{Z}$ $(M\geqslant 2)$
$\mathbb{B}=\mathbb{T}^d$	0	$\mathbb{Z}$	$\mathbb{Z}^3$	$\mathbb{Z}^6$ $(M=1)$ $\mathbb{Z}^7$ $(M\geqslant 2)$

		TRS	PHS	SLS	$d=1$	$d=2$	$d=3$
Standard	A (unitary)	0	0	0	-	$\mathbb{Z}$	-
(Wigner-Dyson)	AI (orthogonal)	+1	0	0	-	-	-
	AII (symplectic)	−1	0	0	-	$\mathbb{Z}_2$	$\mathbb{Z}_2$

Table taken from [SRFL]

$d=3$ The cases $\mathbb{B}=\mathbb{S}^3$ and $\mathbb{B}=\mathbb{T}^3$ are different. In the periodic case one has $\mathbb{Z}^3$ distinct quantum phases. These are three-dimensional versions of a 2D quantum Hall insulators.

		TRS	PHS	SLS	$d=1$	$d=2$	$d=3$
Standard	A (unitary)	0	0	0	-	$\mathbb{Z}$	-
(Wigner-Dyson)	AI (orthogonal)	+1	0	0	-	-	-
	AII (symplectic)	−1	0	0	-	$\mathbb{Z}_2$	$\mathbb{Z}_2$

Table taken from [SRFL]

Let H acts on a space $\mathscr{H}$ and C is a (anti-linear) complex conjugation on $\mathscr{H}$.

Definition (Time Reversal Symmetry)

The Hamiltonian H has a Time Reversal Symmetry (TRS) if there exists a unitary operator U such that:

$$U\,H\,U^* \;=\; C\,H\,C\,.$$

$$H \quad \text{is in class} \quad \begin{cases} \text{AI} & \text{if} \quad CUC = +U^* \qquad \text{(even)} \\ \text{AII} & \text{if} \quad CUC = -U^* \qquad \text{(odd)}\,. \end{cases}$$

Involutions over the Brillouin Zone

Let $\mathbb{B} \ni k \mapsto P_F(k)$ be the fibered Fermi projection of a band insulator H. If H has a TRS, U acts by “reshuffling the fibers”

$$U\, P_F(k)\, U^* \;=\; C\, P_F(\tau(k))\, C \qquad\qquad \forall\, k \in \mathbb{B}.$$

Here $\tau : \mathbb{B} \to \mathbb{B}$ is an involution:

Definition (Involution)

Let X be a topological space and $\tau : X \to X$ a homeomorphism. We said that τ is an involution if $\tau^2 = \mathrm{Id}_X$. The pair (X, τ) is called an involutive space.

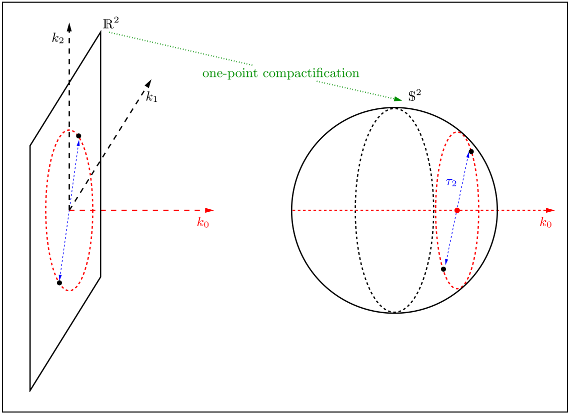
☞ **Remark:** Each space X admits the trivial involution $\tau_{\mathrm{triv}} := \mathrm{Id}_X$.

Continuous case $\mathbb{B} = \mathbb{S}^d$

$$\mathbb{S}^d \xrightarrow{\quad \tau_d \quad} \mathbb{S}^d$$

$$\tilde{\mathbb{S}}^d := (\mathbb{S}^d, \tau_d)$$

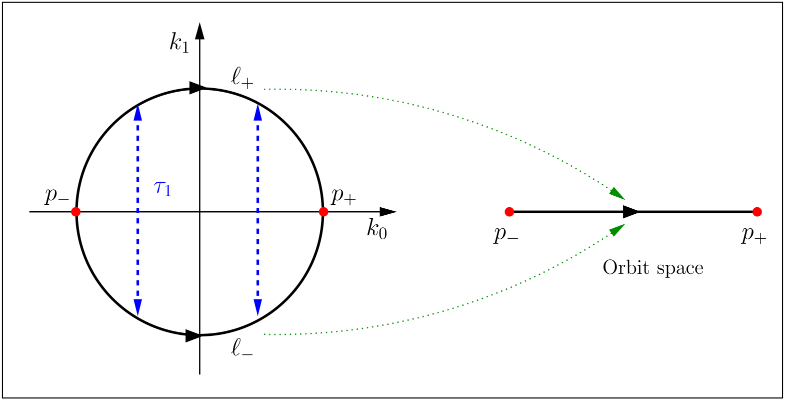
$$(+k_0, +k_1, \ldots, +k_d) \overset{\tau_d}{\longmapsto} (+k_0, -k_1, \ldots, -k_d)$$



Periodic case $\mathbb{B} = \mathbb{T}^d$

$$\mathbb{T}^d = \mathbb{S}^1 \times \ldots \times \mathbb{S}^1 \xrightarrow{\tau_d := \tau_1 \times \ldots \times \tau_1} \mathbb{T}^d = \mathbb{S}^1 \times \ldots \times \mathbb{S}^1$$

$$\tilde{\mathbb{T}}^d := (\mathbb{T}^d, \tau_d)$$



Vector Bundles over Involutive Spaces

$$U\, P_F(k)\, U^* \;=\; C\, P_F(\tau(k))\, C \qquad\qquad \forall\; k \in \mathbb{B}$$

induces an additional structure on the Bloch-bundle $\mathscr{E} \to \mathbb{B}$.

Definition (Atiyah, 1966)

Let (X, τ) be an involutive space and $\mathscr{E} \to X$ an complex vector bundle. Let $\Theta : \mathscr{E} \to \mathscr{E}$ an homeomorphism such that

$$\Theta \;:\; \mathscr{E}|_x \longrightarrow \mathscr{E}|_{\tau(x)} \qquad \text{is anti-linear}\,.$$

- The pair $(\mathscr{E}, \tau)$ is a "Real"-bundle over (X, τ) if

$$\Theta^2 \;:\; \mathscr{E}|_x \xrightarrow{+1} \mathscr{E}|_x \qquad\qquad \forall\; x \in X\,;$$

- The pair $(\mathscr{E}, \tau)$ is a "Quaternionic"-bundle over (X, τ) if

$$\Theta^2 \;:\; \mathscr{E}|_x \xrightarrow{-1} \mathscr{E}|_x \qquad\qquad \forall\; x \in X\,.$$

AZC	TRS	Category	VB
A	0	complex	$\mathrm{Vec}_{\mathbb{C}}^{M}(X)$
AI	$+$	"Real"	$\mathrm{Vec}_{\mathscr{R}}^{M}(X,\tau)$
AII	$-$	"Quaternionic"	$\mathrm{Vec}_{\mathscr{Q}}^{M}(X,\tau)$

The names are justified by the following isomorphisms:

$$\mathrm{Vec}_{\mathscr{R}}^{M}(X,\mathrm{Id}_X) \simeq \mathrm{Vec}_{\mathbb{R}}^{M}(X)$$

$$\mathrm{Vec}_{\mathscr{Q}}^{M}(X,\mathrm{Id}_X) \simeq \mathrm{Vec}_{\mathbb{H}}^{M}(X)$$

The Homotopy Classification ... and Beyond

Gapped band insulator of type A at Fermi energy E_F

$\Updownarrow$

Rank M complex vector bundle over $\mathbb{B}$

$\Updownarrow$

$$\mathrm{Vec}^M_{\mathbb{C}}(\mathbb{B}) \simeq [\mathbb{B}, \mathrm{Gr}_M(\mathbb{C}^N)] \qquad (N \gg 1)$$

Gapped band insulator of type AI at Fermi energy E_F

$\Updownarrow$

Rank M "Real" vector bundle over $\mathbb{B}$

$\Updownarrow$

$$\mathrm{Vec}^M_{\mathscr{R}}(\mathbb{B}, \tau) \simeq [\mathbb{B}, \mathrm{Gr}_M(\mathbb{C}^N)]_{\mathbb{Z}_2} \qquad (N \gg 1)$$

$[\mathbb{B}, \mathrm{Gr}_M(\mathbb{C}^N)]_{\mathbb{Z}_2}$ $\mathbb{Z}_2$-homotopy classes of equivariant maps $f(\tau(k)) = \overline{f(k)}$,
(the Grassmannian is an involutive space w.r.t. the complex conjugation).

– The computation of $[\mathbb{B}, \mathrm{Gr}_M(\mathbb{C}^N)]_{\mathbb{Z}_2}$ is generally extremely difficult.

– Nevertheless, we proved $[\tilde{\mathbb{S}}^1, \mathrm{Gr}_M(\mathbb{C}^N)]_{\mathbb{Z}_2} = 0$ (in $d = 1$ no topology !!).

– We need a new tool like the Peterson's Theorem in the complex case (A)

$$\mathrm{Vec}^M_{\mathbb{C}}(X) \simeq H^2(X, \mathbb{Z}) \qquad \text{if} \quad \dim(X) \leqslant 3\,.$$

Indeed, this extends to the "Real" case (AI) if one "refines" the cohomology.

Theorem (D. & Gomi, 2014)

$$\mathrm{Vec}^M_{\mathscr{R}}(X, \tau) \simeq H^2_{\mathbb{Z}_2}(X, \mathbb{Z}(1)) \qquad \textit{if} \quad \dim(X) \leqslant 3$$

the isomorphism $\mathscr{E} \mapsto \tilde{c}(\mathscr{E})$ is called "Real" (first) Chern class.

– In this case trivial phase $\Leftrightarrow$ exists a global frame of continuous Bloch functions such that $\psi(\tau(k)) = (\Theta\psi)(k)$ ("Real" frame).

The Borel's construction

- (X, τ) any involutive space and $(\mathbb{S}^\infty, \theta)$ the infinite sphere (contractible space) with the antipodal (free) involution:

$$X_{\sim\tau} := \frac{\mathbb{S}^\infty \times X}{\theta \times \tau} \qquad \text{(homotopy quotient)}\,.$$

- $\mathscr{Z}$ any abelian ring (module, system of coefficients, ...)

$$H^j_{\mathbb{Z}_2}(X, \mathscr{Z}) := H^j(X_{\sim\tau}, \mathscr{Z}) \qquad \text{(eq. cohomology groups)}\,.$$

- $\mathbb{Z}(m)$ the $\mathbb{Z}_2$-local system on X based on the module $\mathbb{Z}$

$$\mathbb{Z}(m) \simeq X \times \mathbb{Z} \qquad \text{endowed with} \qquad (x, \ell) \mapsto (\tau(x), (-1)^m \ell)\,.$$

Outline

Theorem (D. & Gomi, 2014)

$$H^2_{\mathbb{Z}_2}(\tilde{\mathbb{S}}^d, \mathbb{Z}(1)) = H^2_{\mathbb{Z}_2}(\tilde{\mathbb{T}}^d, \mathbb{Z}(1)) = 0 \qquad \forall\, d \in \mathbb{N}\,.$$

The proof requires an equivariant generalization of the Gysin sequence and the suspension periodicity.

VB	AZC	$d=1$	$d=2$	$d=3$	$d=4$	
$\mathrm{Vec}^M_{\mathbb{C}}(\mathbb{S}^d)$	**A**	0	$\mathbb{Z}$	0	0 $(M=1)$ $\mathbb{Z}$ $(M\geqslant 2)$	Free
$\mathrm{Vec}^M_{\mathscr{R}}(\tilde{\mathbb{S}}^d)$	**AI**	0	0	0	0 $(M=1)$ $2\mathbb{Z}$ $(M\geqslant 2)$	systems
$\mathrm{Vec}^M_{\mathbb{C}}(\mathbb{T}^d)$	**A**	0	$\mathbb{Z}$	$\mathbb{Z}^3$	$\mathbb{Z}^6$ $(M=1)$ $\mathbb{Z}^7$ $(M\geqslant 2)$	Periodic
$\mathrm{Vec}^M_{\mathscr{R}}(\tilde{\mathbb{T}}^d)$	**AI**	0	0	0	0 $(M=1)$ $2\mathbb{Z}$ $(M\geqslant 2)$	systems

Outline

The case $d = 4$ is interesting for the magneto-electric response (space-time variables) [QHZ,HPB]

Theorem (D. & Gomi, 2014)

Class AI topological insulators in $d = 4$ are completely classified by the 2-nd "Real" Chern class. These classes are representable as even integers and the isomorphisms

$$\mathrm{Vec}^{M}_{\mathscr{R}}(\tilde{\mathbb{T}}^4) \simeq 2\mathbb{Z}\,, \qquad \mathrm{Vec}^{M}_{\mathscr{R}}(\tilde{\mathbb{S}}^4) \simeq 2\mathbb{Z}$$

are given by the (usual) 2-nd Chern number.

☞ **Remark:** In $d = 4$ to have an even 2-nd Chern number is a necessary condition for a complex vector bundle to admit a "Real"-structure **!!**

Models for Non-Trivial Phases

$$H := \sum_{j=0}^{4} f_j(-\mathrm{i}\partial_{x_1}, \ldots, -\mathrm{i}\partial_{x_4}) \otimes \Sigma_j \qquad \text{on} \qquad L^2(\mathbb{R}^4) \otimes \mathbb{C}^4 \,.$$

- $\{\Sigma_j\}_{j=0,1,\ldots,4}$ is a Clifford basis such that

$$\Sigma_j^* = \Sigma_j \,, \qquad \overline{\Sigma_j} = (-1)^j \, \Sigma_j \,, \qquad \Sigma_0 \, \Sigma_1 \, \Sigma_2 \, \Sigma_3 \, \Sigma_4 \; = \; -\mathbb{1}_4 \,;$$

- $f_j : \mathbb{R}^4 \to \mathbb{R}$ are bounded functions such that

$$f_j(-k) = \varepsilon_j \, f_j(k) \,, \qquad k \in \mathbb{R}^4 \quad \varepsilon_j \in \{-1, +1\} \,.$$

- $U := \mathbb{1} \otimes \Theta$ with $\Theta \in \{\mathbb{1}_4, \Sigma_0, \Sigma_2, \Sigma_4\}$

Θ	ε_0	ε_1	ε_2	ε_3	ε_4	
$\mathbb{1}_4$	$+$	$-$	$+$	$-$	$+$	**AI**
Σ_0	$+$	$+$	$-$	$+$	$-$	
Σ_2	$-$	$+$	$+$	$+$	$-$	
Σ_4	$-$	$+$	$-$	$+$	$+$	

Thank you for your attention

Recommended Bibliography

Classification of Topological Insulators:

[Ki] Kitaev, A.: AIP Conf. Proc. **1134**, 22-30 (2009)

[SRFL] Schnyder, A.; Ryu, S.; Furusaki, A. & Ludwig, A.: Phys. Rev. B **78**, 195125 (2008)

Topology:

[At] Atiyah, M. F.: Quart. J. Math. Oxford Ser. (2) **17**, 367-386 (1966)

[Bo] Bott, R.: Ann. of Math. **70**, 313-337 (1959)

[Pe] Peterson, F. P.: Ann. of Math. **69**, 414-420 (1959)

Magneto-electric Response:

[HPB] Hughes, T. L.; Prodan, E.; Bernevig, B. A.: Phys. Rev. B **83**, 245132 (2011)

[QHZ] Qi, X.-L.; Hughes, T. L.; Zhang, S.-C.: Phys. Rev. B **78**, 195424 (2008)