1) Band theory and Atiyah-Hirzebruch spectral sequence

2) Space group and topological invariants in band theory

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Plan

- Atiyah-Hirzebruch Spectral Sequence in K-theory
- E_∞-page of Class A and AIII
- New topological invariants

Ref

KS, M. Sato, K. Gomi, arXiv:1802.06694

Related prior works

Compatibility relation, Symmetry-based indicator, ...
- Kruthoff, Boer, Wezel, Kane, Slager
- Po, Vishwanath, Watanabe
- Bradlyn, Elcoro, Cano, Vergniory, Wang, Felser, Aroyo, Bernevig
- C.Fang, Song, Zhang, Z.Fang

Atiyah-Hirzebruch Spectral Sequence (AHSS)

- The AHSS [Atiyah-Hirzebruch '61] is a spectral sequence to compute a generalized (co)homology theory h^*.
- For the band topology, the cohomology theory is the twisted equivariant K-theory ${}^{\phi}K_G^{(\tau,c)-n}(X)$ by Freed and Moore.
- Today, I focus on class A and AIII band insulators with space group symmetry.
- The following formulation does apply to any symmetry classes in band theory.
- The AHSS is the perfect generalization of the compatibility relation in band theory.

Notation

- The K-group is written as

$$K_G^{\tau-n}(X) = \begin{cases} K_G^{\tau-0}(X) & (n \in \text{even : class A}) \\ K_G^{\tau-1}(X) & (n \in \text{odd : class AIII}) \end{cases}$$

- X is a BZ manifold (momentum space).
- G is a point group acting on X.
- τ represents the factor system and nonprimitive lattice translations.
- Meaning I: The classification of gapped Hamiltonians over X with symmetry G in the AZ class n.
- Meaning II: The classification of gapless Hamiltonians over X with symmetry G in the AZ class $(n+1)$.
- Bott periodicity (complex AZ classes)

$$K_G^{\tau-n+2}(X) \cong K_G^{\tau-n}(X).$$

Cell decomposition

- We want to compute the K-group $K_G^{\tau-n}(X)$, the classification of band insulators over the BZ X.
- Introduce a G-symmetric cell decomposition of the d-dimensional BZ X.

$$X = \{0\text{-cells}\} \sqcup \{1\text{-cells}\} \sqcup \{2\text{-cells}\} \sqcup \cdots$$

- Each p-cell is a p-dimensional open disc D^p.
- This gives a filtration of X,

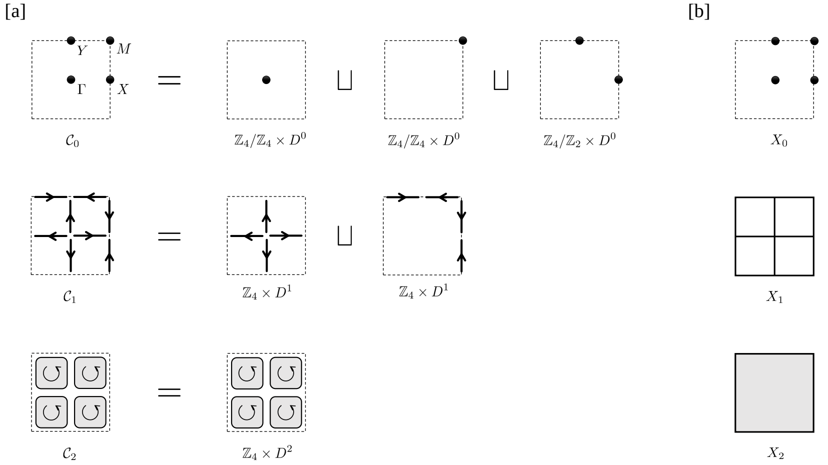
$$X_0 \subset X_1 \subset \cdots X_{d-1} \subset X_d = X,$$

where the p-skeleton X_p is defined as

$$X_0 = \{0\text{-cells}\}, \qquad X_p = X_{p-1} \cup \{p\text{-cells}\}.$$

Cell decomposition

Ex: 2d BZ with C_4-rotation symmetry.



E_1-page

- The E_1-page is defined as

$$\begin{aligned} E_1^{p,-n} &:= K_G^{\tau+p-n}(X_p, X_{p-1}) \\ &\cong \prod_{j \in p\text{-cells}} K_{G_j}^{\tau_j+p-n}(D_j^p, \partial D_j^p) \\ &\cong \prod_{j \in p\text{-cells}} \widetilde{K}_{G_j}^{\tau_j+p-n}(D_j^p / \partial D_j^p) \\ &\cong \prod_{j \in p\text{-cells}} K_{G_j}^{\tau_j-n}(D_j^p) \qquad (\because \text{suspension iso.}) \end{aligned}$$

- Here, the relative K-group $K_G^{\tau-n}(X, Y)$, $Y \subset X$, means Hamiltonians over X which are trivial over Y.
- $D_j^p(\sim pt)$ are p-cells (p-dim. open discs) labeled by j.
- $G_j \subset G$ is the little group on the p-cell D_j^p, i.e. $g\boldsymbol{k} = \boldsymbol{k}$ for $\boldsymbol{k} \in D_j^p, g \in G_j$.
- τ_j is the factor system on the p-cell D_j^p.

E_1-page

- $E_1^{p,-n} = \prod_{j \in p\text{-cells}} K_{G_j}^{\tau_j - n}(D_j^p)$ is easily determined, since $K_{G_j}^{\tau_j - n}(D_j^p)$ is just the K-group over a point.

$$K_{G_j}^{\tau_j - n}(D_j^p) = \begin{cases} \mathbb{Z}^{\oplus(\#\text{ of irreps at } D_j^p)} & n \in \mathrm{even} \quad \text{(class A)} \\ 0 & n \in \mathrm{odd} \quad \text{(class AIII)} \end{cases}$$

A	$n=-2$	$\mathbb{Z}^{n_0}$	$\mathbb{Z}^{n_1}$	$\mathbb{Z}^{n_2}$	$\mathbb{Z}^{n_3}$
AIII	$n=-1$	0	0	0	0
A	$n=0$	$\mathbb{Z}^{n_0}$	$\mathbb{Z}^{n_1}$	$\mathbb{Z}^{n_2}$	$\mathbb{Z}^{n_3}$
AIII	$n=1$	0	0	0	0
A	$n=2$	$\mathbb{Z}^{n_0}$	$\mathbb{Z}^{n_1}$	$\mathbb{Z}^{n_2}$	$\mathbb{Z}^{n_3}$
AIII	$n=3$	0	0	0	0
	$E_1^{p,-n}$	$p=0$	$p=1$	$p=2$	$p=3$

E_1-page

The E_1-page has multiple meanings.

Meaning of the E^1-page as class A:

- $E_1^{p,-p} = \prod_{j \in p\text{-cells}} K_{G_j}^{\tau_j+0}(D_j^p, \partial D_j^p)$: Class A topological insulators on p-cells D_j^p which are trivial on the boundary ∂D_j^p.
- $E_1^{p,1-p} = \prod_{j \in p\text{-cells}} K_{G_j}^{\tau_j+1}(D_j^p, \partial D_j^p)$: Class A gapless points on p-cells D_j^p which are gapped on the boundary ∂D_j^p.

A	$n=-2$	$\mathbb{Z}^{n_0}$	$\mathbb{Z}^{n_1}$	$\mathbb{Z}^{n_2}$	$\mathbb{Z}^{n_3}$
AIII	$n=-1$	0	0	0	0
A	$n=0$	$\mathbb{Z}^{n_0}$	$\mathbb{Z}^{n_1}$	$\mathbb{Z}^{n_2}$	$\mathbb{Z}^{n_3}$
AIII	$n=1$	0	0	0	0
A	$n=2$	$\mathbb{Z}^{n_0}$	$\mathbb{Z}^{n_1}$	$\mathbb{Z}^{n_2}$	$\mathbb{Z}^{n_3}$
AIII	$n=3$	0	0	0	0
	$E_1^{p,-n}$	$p=0$	$p=1$	$p=2$	$p=3$

- In addition, the E_1-page represents *singular points*. See [arXiv:1802.06694] for the detail.

E_1-page

Meaning of the E^1-page as class AIII:

- $E_1^{p,1-p} = \prod_{j \in p\text{-cells}} K_{G_j}^{\tau_j+1}(D_j^p, \partial D_j^p)$: Class AIII topological insulators on p-cells D_j^p which are trivial on the boundary ∂D_j^p.
- $E_1^{p,2-p} = \prod_{j \in p\text{-cells}} K_{G_j}^{\tau_j+2}(D_j^p, \partial D_j^p)$: Class AIII gapless points on p-cells D_j^p which are gapped on the boundary ∂D_j^p.

A	$n=-2$	$\mathbb{Z}^{n_0}$	$\mathbb{Z}^{n_1}$	$\mathbb{Z}^{n_2}$	$\mathbb{Z}^{n_3}$
AIII	$n=-1$	0	0	0	0
A	$n=0$	$\mathbb{Z}^{n_0}$	$\mathbb{Z}^{n_1}$	$\mathbb{Z}^{n_2}$	$\mathbb{Z}^{n_3}$
AIII	$n=1$	0	0	0	0
A	$n=2$	$\mathbb{Z}^{n_0}$	$\mathbb{Z}^{n_1}$	$\mathbb{Z}^{n_2}$	$\mathbb{Z}^{n_3}$
AIII	$n=3$	0	0	0	0
	$E_1^{p,-n}$	$p=0$	$p=1$	$p=2$	$p=3$

1st differential d_1

- The 1st differential

$$d_1^{p,-n} : E_1^{p,-n} \to E_1^{p+1,-n}$$

is defined as the following process:

(i) Change a topological invariant of topological insulator $x \in E_1^{p,-n}$ on a p-cell D_j^p.

(ii) Then, the pair-creation of gapless points occurs in the adjacent $(p+1)$-cells D_j^{p+1}, which changes the topological charge of gapless points in the adjacent $(p+1)$-cell D_j^{p+1} by $d_1^{p,-n}(x) \in E_1^{p+1,-n}$.

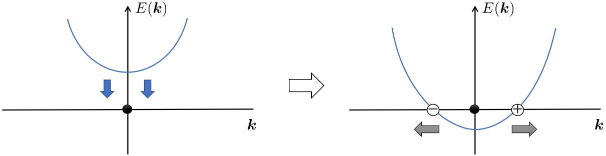
- It follows that $d_1 \circ d_1 = 0$. $\Rightarrow$ cohomology of d_1

A	$n=0$	$\mathbb{Z}^{n_0}$	$\to$	$\mathbb{Z}^{n_1}$	$\to$	$\mathbb{Z}^{n_2}$	$\to$	$\mathbb{Z}^{n_3}$
AIII	$n=1$	0	$\to$	0	$\to$	0	$\to$	0
A	$n=2$	$\mathbb{Z}^{n_0}$	$\to$	$\mathbb{Z}^{n_1}$	$\to$	$\mathbb{Z}^{n_2}$	$\to$	$\mathbb{Z}^{n_3}$
AIII	$n=3$	0	$\to$	0	$\to$	0	$\to$	0
	$E_1^{p,-n}$	$p=0$		$p=1$		$p=2$		$p=3$

Ex: 1st differential $d_1^{0,0}$ (compatibility relation)

- $d_1^{0,0} : E_1^{0,0} \to E_1^{1,0}$
- Change the number of class A irreps at a 0-cell and create a fermi surface in adjacent 1-cells.
- This is so called the compatibility relation.
- The compatibility relations from $p(>0)$-cells to $(p+1)$-cells follow from $d_1^{0,0}$ because $d_1 \circ d_1 = 0$.

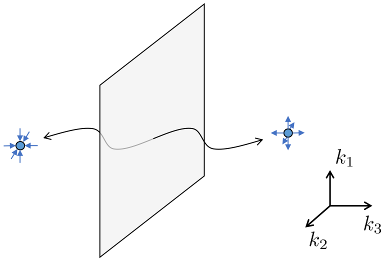
A	$n=0$	$\mathbb{Z}^{n_0} \xrightarrow{d_1^{0,0}}$	$\mathbb{Z}^{n_1}$	$\mathbb{Z}^{n_2}$	$\mathbb{Z}^{n_3}$
AIII	$n=1$	0	0	0	0
A	$n=2$	$\mathbb{Z}^{n_0}$	$\mathbb{Z}^{n_1}$	$\mathbb{Z}^{n_2}$	$\mathbb{Z}^{n_3}$
AIII	$n=3$	0	0	0	0
	$E_1^{p,-n}$	$p=0$	$p=1$	$p=2$	$p=3$



Ex: 1st differential $d_1^{2,-2}$

- $d_1^{2,-2} : E_1^{2,-2} \to E_1^{3,-2}$
- Change the class A Chern number on 2-cells and create Weyl points in adjacent 3-cells.

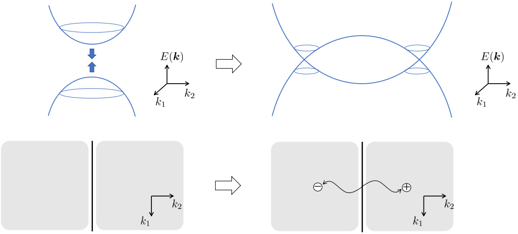
A	$n=0$	$\mathbb{Z}^{n_0}$	$\mathbb{Z}^{n_1}$	$\mathbb{Z}^{n_2}$	$\mathbb{Z}^{n_3}$
AIII	$n=1$	0	0	0	0
A	$n=2$	$\mathbb{Z}^{n_0}$	$\mathbb{Z}^{n_1}$	$\mathbb{Z}^{n_2} \xrightarrow{d_1^{2,-2}}$	$\mathbb{Z}^{n_3}$
AIII	$n=3$	0	0	0	0
	$E_1^{p,-n}$	$p=0$	$p=1$	$p=2$	$p=3$



Ex: 1st differential $d_1^{1,-1}$

- $d_1^{1,-1} : E_1^{1,-1} \to E_1^{2,-1}$
- Change the class AIII winding number on 1-cells and create Dirac points in adjacent 2-cells.

A	$n=0$	$\mathbb{Z}^{n_0}$	$\mathbb{Z}^{n_1}$	$\xrightarrow{d_1^{1,-1}}$	$\mathbb{Z}^{n_2}$	$\mathbb{Z}^{n_3}$
AIII	$n=1$	0	0		0	0
A	$n=2$	$\mathbb{Z}^{n_0}$	$\mathbb{Z}^{n_1}$		$\mathbb{Z}^{n_2}$	$\mathbb{Z}^{n_3}$
AIII	$n=3$	0	0		0	0
	$E_1^{p,-n}$	$p=0$	$p=1$		$p=2$	$p=3$



E_2-page

- Because $d_1 \circ d_1 = 0$, one can take the cohomology of d_1. It gives the E_2-page

$$E_2^{p,-n} := \text{Ker } d_1^{p,-n} / \text{Im } d_1^{p-1,-n}.$$

- The meaning of the E_2-page: Hamiltonians in p-cells which can not be trivialized by adjacent $(p-1)$-cells and can extend to adjacent $(p+1)$-cells.
- A comment: $E_2^{0,0}$ for all the 1651 magnetic space groups were computed in Watanabe-Po-Vishwanath.

E_r-page and r-th differential d_r

- This is not the end of story.
- There exist "higher order" compatibility relations.
- The r-th differential

$$d_r : E_r^{p,-n} \to E_r^{p+r,-n-r+1}$$

is defined as

(i) Change a topological invariant of topological insulator $x \in E_r^{p,-n}$ on p-cells. Typically, this is the band inversion at high-symmetric points.

(ii) Then, the pair-creation of gapless points occurs in the adjacent $(p+r)$-cells, which changes the topological charge of gapless points in the adjacent $(p+r)$-cells by $d_r^{p,-n}(x) \in E_r^{p+r,-n-r+1}$.

- The E_{r+1}-page is defined to be the cohomology of d_r

$$E_{r+1}^{p,-n} = \mathrm{Ker}\ d_r^{p,-n} / \mathrm{Im}\ d_r^{p-r,-n+r-1}.$$

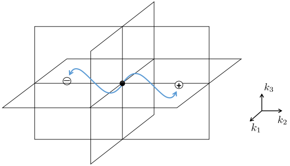
Ex: 3rd differential $d_3^{0,0}$

- $d_3^{0,0} : E_3^{0,0} \to E_3^{3,-2}$
- Band inversion at a 0-cell and creating Weyl points in adjacent 3-cells.
- Ex: 3d with inversion symmetry (space group P$\bar{1}$).

$$d_3^{0,0} : \mathbb{Z}^9 \to \mathbb{Z}_2, \qquad \{n_{\text{total}}, \{n_\Gamma^-\}\} \mapsto \sum_{\Gamma \in \text{h.s.p.}} n_\Gamma^- \mod 2.$$

A	$n=0$	$\mathbb{Z}^9$	0	$\mathbb{Z}^3$	$\mathbb{Z}_2$
AIII	$n=1$	0	0	0	0
A	$n=2$	$\mathbb{Z}^9$	0	$\mathbb{Z}^3$	$\mathbb{Z}_2$
AIII	$n=3$	0	0	0	0
	$E_3^{p,-n}$	$p=0$	$p=1$	$p=2$	$p=3$

$d_3^{0,0}$



- The nontriviality of $d_3^{0,0}$ implies that (i) the total inversion parity should be even in class A insulators [Turner-Zhang-Mong-Vishwanath].

E_∞-page

- When X is d-dimensional, the E_r-page converges at $r = d + 1$.

$$E_1 \Rightarrow E_2 \Rightarrow \cdots E_d \Rightarrow E_{d+1} = E_{d+2} = \cdots =: E_\infty.$$

- The limiting page is called E_∞-page.
- The meaning of the E_∞-page: Hamiltonians in p-cells which can not be trivialized by adjacent low-dimensional cells and can extend to adjacent high-dimensional cells.
- In principle, one can compute the E_∞-page for a given symmetry class.
- The E_∞-page approximates the K-group $K_G^{\tau-n}(X)$ as follows.

E_∞-page

- Introduce subgroups $F^pK^{-n} \subset K_G^{\tau-n}(X), p = 0, \dots d$, by

$$F^pK^{-n} := \mathrm{Ker}\,[i^* : K_G^{\tau-n}(X) \to K_G^{\tau|_{X_{p-1}}-n}(X_{p-1})],$$

where $i : X_{p-1} \to X$ is the inclusion and i^* is pull-back.

- F^pK^{-n} means Hamiltonians on X which are trivial on X_{p-1}.
- F^pK^{-n} gives the filtration of $K_G^{\tau-n}(X)$ as

$$0 \subset F^dK^{-n} \subset F^{d-1}K^{-n} \subset \cdots F^2K^{-n} \subset F^1K^{-n} \subset K_G^{\tau-n}(X).$$

- The key is that the quotient is the E_∞-page

$$E_\infty^{p,-p-n} = F^pK^{-n}/F^{p+1}K^{-n}$$

$\because$ The r.h.s. represents Hamiltonians which are trivial on X_p but nontrivial on X_{p+1}. This is the same meaning of the l.h.s.

E_∞-page

- Ex: d=3.

$$0 \longrightarrow F^1K^{-n} \longrightarrow K_G^{\tau-n}(X) \longrightarrow E_\infty^{0,-n} \longrightarrow 0,$$
$$0 \longrightarrow F^2K^{-n} \longrightarrow F^1K^{-n} \longrightarrow E_\infty^{1,-1-n} \longrightarrow 0,$$
$$0 \longrightarrow E_\infty^{3,-3-n} \longrightarrow F^2K^{-n} \longrightarrow E_\infty^{2,-2-n} \longrightarrow 0.$$

E_∞-page for class A and AIII

- Our main result is to give the complete list of the E_∞-pages for all the 230 space groups in class A and AIII.

No.		$E_\infty^{0,\mathrm{even}}$	$E_\infty^{1,\mathrm{even}}$	$E_\infty^{2,\mathrm{even}}$	$E_\infty^{3,\mathrm{even}}$
1	$P1$	$\mathbb{Z}$	$\mathbb{Z}^3$	$\mathbb{Z}^3$	$\mathbb{Z}$
2	$P\bar{1}$	$\mathbb{Z}^9$	0	$\mathbb{Z}^3$	0
3	$P2$	$\mathbb{Z}^5$	$\mathbb{Z}^5$	$\mathbb{Z}$	$\mathbb{Z}$
⋮					
230, spinless	$Ia\bar{3}d$	$\mathbb{Z}^9$	0	0	0
230, spinful	$Ia\bar{3}d$	$\mathbb{Z}^7$	$\mathbb{Z}$	0	0

- For class A insulators, $E_\infty^{0,\mathrm{even}}$ are free. The K-groups as abelian groups are given as

$$K_G^{\tau-0}(T^3) \cong E_\infty^{2,\mathrm{even}} \oplus E_\infty^{0,\mathrm{even}}.$$

- For class AIII insulators, the K-groups fit into the short exact sequence

$$0 \to E_\infty^{3,\mathrm{even}} \to K_G^{\tau-1}(T^3) \to E_\infty^{1,\mathrm{even}} \to 0.$$

Summary

- We found that the Atiyah-Hirzebruch spectral sequence (AHSS) is a very efficient tool to study the band topology.
- The differentials d_r in the AHSS are understood as the generalization of the compatibility relation.
- The E_∞-page approximates the K-group.
- We have computed the complete list of the E_∞-page for class A and AIII.
- With (magnetic)space group symmetry there are many unrevealed torsion topological invariants beyond the periodic table by Schnyder-Ryu-Furusaki-Ludwig and Kitaev.

New topological invariants

- We found that there are many torsion topological invariants in class A and AIII.
- Some exs (very selective):

No.		$E_\infty^{0,\mathrm{even}}$	$E_\infty^{1,\mathrm{even}}$	$E_\infty^{2,\mathrm{even}}$	$E_\infty^{3,\mathrm{even}}$
7	Pc	$\mathbb{Z}$	$\mathbb{Z}^2 + \mathbb{Z}_2$	$\mathbb{Z} + \mathbb{Z}_2$	0
$16, \mathrm{spinless}$	$P222$	$\mathbb{Z}^{13}$	$\mathbb{Z}_2$	0	$\mathbb{Z}$
19	$P2_12_12_1$	$\mathbb{Z}$	$\mathbb{Z}_4^3$	0	$\mathbb{Z}$
$22, \mathrm{spinless}$	$F222$	$\mathbb{Z}^7$	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$
144	$P3_1$	$\mathbb{Z}$	$\mathbb{Z} + \mathbb{Z}_3^2$	$\mathbb{Z}$	$\mathbb{Z}$
169	$P6_1$	$\mathbb{Z}$	$\mathbb{Z} + \mathbb{Z}_6$	$\mathbb{Z}$	$\mathbb{Z}$

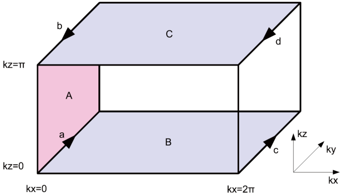
- See [arXiv:1802.06694] for the explicit constructions of some torsion topological invariants.

Ex: No.7 (Pc: primitive cubic, glide reflection)

No.		$E_\infty^{0,\mathrm{even}}$	$E_\infty^{1,\mathrm{even}}$	$E_\infty^{2,\mathrm{even}}$	$E_\infty^{3,\mathrm{even}}$
7	Pc	$\mathbb{Z}$	$\mathbb{Z}^2 + \mathbb{Z}_2$	$\mathbb{Z} + \mathbb{Z}_2$	0

- There is a $\mathbb{Z}_2$ topological invariant in class A insulators defined on the 2-skeleton X_2.
- C_s-symmetric cell decomposition of the BZ:

$$\frac{\mathrm{BZ}}{2} =$$



- Explicit form of the $\mathbb{Z}_2$ invariant.[Fang-Fu, KS-Sato-Gomi]

$$(-1)^{\nu} := \exp\left[\frac{1}{2}\int_A \mathcal{F} - \oint_a \mathcal{A} - \oint_b \mathcal{A}\right].$$

Ex: No.22 (F222: face-centered cubic, D_2)

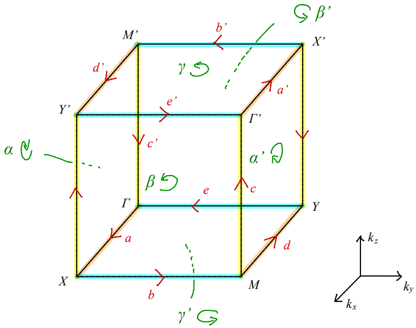
No.		$E_\infty^{0,\mathrm{even}}$	$E_\infty^{1,\mathrm{even}}$	$E_\infty^{2,\mathrm{even}}$	$E_\infty^{3,\mathrm{even}}$
22, spinless	$F222$	$\mathbb{Z}^7$	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$
22, spinful	$F222$	$\mathbb{Z}$	$\mathbb{Z}^6$	$\mathbb{Z}_2$	$\mathbb{Z}$

- There is a $\mathbb{Z}_2$ topological invariant in class A insulators defined on the 2-skeleton X_2.
- Reciprocal lattice vectors (in the unit of 2π): $b_1 = (-1, 1, 1), b_2 = (1, -1, 1), b_3 = (1, 1, -1)$.
- D_2 symmetry: $D_2 = \{1, 2_{100}, 2_{010}, 2_{001}\}$,

$$\begin{cases} 2_{100} : (x, y, z) \mapsto (x, -y, -z), \\ 2_{010} : (x, y, z) \mapsto (-x, y, -z), \\ 2_{001} : (x, y, z) \mapsto (-x, -y, z). \end{cases}$$

- D_2-symmetric cell decomposition of the BZ:

$$\frac{\mathrm{BZ}}{4} =$$



- The boundary of $BZ/4$ is found to be the real projective plane:

$$\alpha' = 2_{010}\alpha + b_1 + b_2 + b_3, \quad \beta' = 2_{100}\beta + b_1, \quad \gamma' = 2_{001}\gamma + b_3.$$

- The $\mathbb{Z}_2$ invariant ($\because$ Stokes' formula):

$$(-1)^\nu := \exp\left[\oint_{a+b+c} \mathrm{tr}\,\mathcal{A} - \frac{1}{2}\int_{\alpha+\beta+\gamma} \mathrm{tr}\,\mathcal{F}\right].$$

Ex: No.16 (P222: primitive cubic, D_2), spinless

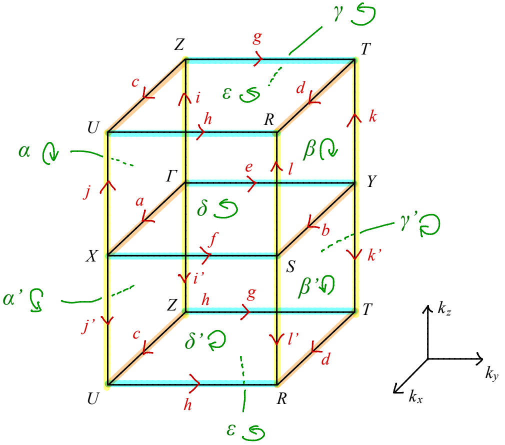
No.		$E_\infty^{0,\mathrm{even}}$	$E_\infty^{1,\mathrm{even}}$	$E_\infty^{2,\mathrm{even}}$	$E_\infty^{3,\mathrm{even}}$
16, spinless	$P222$	$\mathbb{Z}^{13}$	$\mathbb{Z}_2$	0	$\mathbb{Z}$

- There is a $\mathbb{Z}_2$ topological invariant in class AIII insulators defined on the 1-skeleton X_1.
- Reciprocal lattice vectors (in the unit of 2π): $b_1 = (1,0,0), \quad b_2 = (0,1,0), \quad b_3 = (0,0,1)$.
- D_2 symmetry: $D_2 = \{1, 2_{100}, 2_{010}, 2_{001}\}$,

$$\begin{cases} 2_{100} : (x,y,z) \mapsto (x,-y,-z), \\ 2_{010} : (x,y,z) \mapsto (-x,y,-z), \\ 2_{001} : (x,y,z) \mapsto (-x,-y,z). \end{cases}$$

- D_2-symmetric cell decomposition of the BZ:

$$\frac{\mathrm{BZ}}{4} =$$



- $\mathbb{Z}_2$ invariant ??

- A class AIII insulator can be described by a unitary matrix $q(\boldsymbol{k}) \in U(N)$.
- Decomposition per irreps:

$$q(\boldsymbol{k} \in \text{line}) = \begin{pmatrix} q_A(\boldsymbol{k}) & \\ & q_B(\boldsymbol{k}) \end{pmatrix},$$

$$q(\boldsymbol{k} \in \text{point}) = \begin{pmatrix} q_A(\boldsymbol{k}) & & & \\ & q_{B_1}(\boldsymbol{k}) & & \\ & & q_{B_2}(\boldsymbol{k}) & \\ & & & q_{B_3}(\boldsymbol{k}) \end{pmatrix}.$$

  Here, $\{A, B\}$ and $\{A, B_1, B_2, B_3\}$ are irreps. for $\mathbb{Z}_2$ and $D_2 \cong \mathbb{Z}_2 \times \mathbb{Z}_2$, respectively.
- With this structure, one can construct the $\mathbb{Z}_2$ invariant.
- We write $e^{i\theta_{A/B}(\boldsymbol{k})} = \det q_{A/B}(\boldsymbol{k})$ for $\boldsymbol{k}$ $\in$lines and $e^{i\phi_{A/B_i}(\boldsymbol{k})} = \det q_{A/B_i}(\boldsymbol{k})$ for $\boldsymbol{k}$ $\in$points.

- The key point is that the $U(1)$ phases $e^{i\theta_{A/B}(\boldsymbol{k})}$ on lines determines the $U(1)$ phases $e^{i\phi_{A/B_i}(\boldsymbol{k})}$ at points up to a sign ± 1.
- In fact, around the Γ point, the compatibility relation gives the constraint

$$\begin{cases} e^{i\theta_B(\boldsymbol{k}\in a)}\Big|_{\boldsymbol{k}\to\Gamma} = e^{i\phi_{B_1}(\Gamma)+i\phi_{B_2}(\Gamma)}, \\ e^{i\theta_B(\boldsymbol{k}\in e)}\Big|_{\boldsymbol{k}\to\Gamma} = e^{i\phi_{B_1}(\Gamma)+i\phi_{B_3}(\Gamma)}, \\ e^{i\theta_B(\boldsymbol{k}\in i)}\Big|_{\boldsymbol{k}\to\Gamma} = e^{i\phi_{B_2}(\Gamma)+i\phi_{B_2}(\Gamma)}, \end{cases}$$

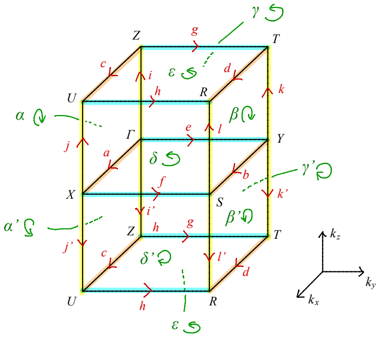
leading to

$$\begin{cases} e^{2i\phi_{B_1}(\Gamma)} = e^{i\theta_B(\boldsymbol{k}\in a)+i\theta_B(\boldsymbol{k}\in e)-i\theta_B(\boldsymbol{k}\in i)}\Big|_{\boldsymbol{k}\to\Gamma}, \\ e^{2i\phi_{B_2}(\Gamma)} = e^{i\theta_B(\boldsymbol{k}\in a)-i\theta_B(\boldsymbol{k}\in e)-i\theta_B(\boldsymbol{k}\in i)}\Big|_{\boldsymbol{k}\to\Gamma}, \\ e^{2i\phi_{B_3}(\Gamma)} = e^{-i\theta_B(\boldsymbol{k}\in a)+i\theta_B(\boldsymbol{k}\in e)-i\theta_B(\boldsymbol{k}\in i)}\Big|_{\boldsymbol{k}\to\Gamma}. \end{cases}$$

- The $\mathbb{Z}_2$ invariant is defined as

$$(-1)^{\nu} := \exp\left[\frac{i}{2}\int_{a-b-c+d-e+f+g-h-i+j+k-\ell} d\theta_B(\boldsymbol{k}) + i\sum_{\boldsymbol{k}\in\Gamma,S,U,T}\phi_{B_3}(\boldsymbol{k}) - i\sum_{\boldsymbol{k}\in X,Y,Z,R}\phi_{B_3}(\boldsymbol{k})\right].$$

$$\frac{\mathrm{BZ}}{4} =$$

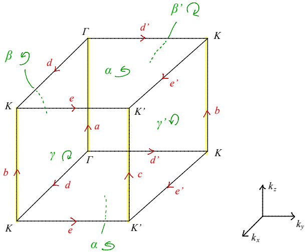


Ex: Screw axis and $\mathbb{Z}_n$ topological invariants in class AIII

No.		$E_\infty^{0,\text{even}}$	$E_\infty^{1,\text{even}}$	$E_\infty^{2,\text{even}}$	$E_\infty^{3,\text{even}}$
4	$P2_1$	$\mathbb{Z}$	$\mathbb{Z}_2^3$	$\mathbb{Z}$	$\mathbb{Z}$
76	$P4_1$	$\mathbb{Z}$	$\mathbb{Z} \times \mathbb{Z}_2 \times \mathbb{Z}_4$	$\mathbb{Z}$	$\mathbb{Z}$
144	$P3_1$	$\mathbb{Z}$	$\mathbb{Z} \times \mathbb{Z}_3^2$	$\mathbb{Z}$	$\mathbb{Z}$
169	$P6_1$	$\mathbb{Z}$	$\mathbb{Z} \times \mathbb{Z}_6$	$\mathbb{Z}$	$\mathbb{Z}$

- For class AIII, there is a $\mathbb{Z}_n$ invariant in the presence of the n-fold screw axis.
- Ex: BZ for $P3_1$:

$$\frac{\mathrm{BZ}}{3} =$$



- On a n-fold screw axis, a class AIII Hamiltonian $q(k_z) \in U(N)$ is decomposed as

$$
\begin{aligned}
q(k_z) &= q_0(k_z) \oplus q_1(k_z) \oplus \cdots \oplus q_{n-1}(k_z), \\
q_p(k_z + 2\pi) &= q_{p+1}(k_z),
\end{aligned}
$$

with respect to the eigenvalues $\lambda_p(k_z) = e^{-i(k_z+2\pi p)/n}$ $(p = 0, 1, \dots, n-1)$.

- Introduce a $U(1)$-valued quantity

$$
e^{i\phi(k_z)} := \det q_0(k_z) \cdot \exp \left[\sum_{p=0}^{n-2} \frac{n-p-1}{n} \int_{k_z}^{k_z+2\pi} d_{k_z} \log \det q_p(k_z) \right]
$$

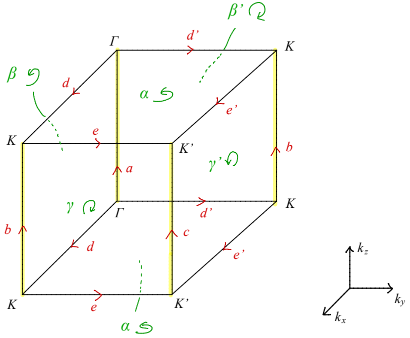
- The nth power is the total determinant

$$
e^{in\phi(k_z)} = \det q(k_z).
$$

- A pair of n-fold axes (X, k_z) and (Y, k_z) gives a $\mathbb{Z}_n$ invariant

$$e^{2\pi i\nu/n} := \exp\Bigg[i\phi(X, k_z) - i\phi(Y, k_z) - \frac{1}{n}\int_{X\to Y} d\boldsymbol{k}\cdot\boldsymbol{\nabla}\log\det q(\boldsymbol{k}, k_z)\Bigg]$$

$$\frac{\mathrm{BZ}}{3} =$$



Summary

- There are many unrevealed topological invariants in band topology.
- The Atiyah-Hirzebruch spectral sequence systematically computes how many topological invariants there are for a given symmetry class.
- The construction of topological invariants looks case by case problems.