Topology from band representations

Jennifer Cano

Stony Brook University and
Flatiron Institute for Computational Quantum Physics

Part 2: Disconnected EBRs

Refs:

“Topological quantum chemistry,” Bradlyn, Elcoro, Cano, Vergniory, Wang, Felser, Aroyo, Bernevig, ArXiv: 1703.02050, Nature 547, 298 — 305 (2017)

“Building blocks of topological quantum chemistry,” Cano, Bradlyn, Wang, Elcoro, Vergniory, Felser, Aroyo, Bernevig ArXiv: 1709.01935, PRB 97, 035139 (2018); Sec IV

“Band connectivity for topological quantum chemistry: band structures as a graph theory problem,” Bradlyn, Elcoro, Vergniory, Cano, Wang, Felser, Aroyo, Bernevig, ArXiv: 1709.01937, PRB 97, 035138 (2018)

“Graph theory data for topological quantum chemistry,” Vergniory, Elcoro, Wang, Cano, Felser, Aroyo, Bernevig, Bradlyn, ArXiv: 1706.08529, PRE 96, 023310 (2017)

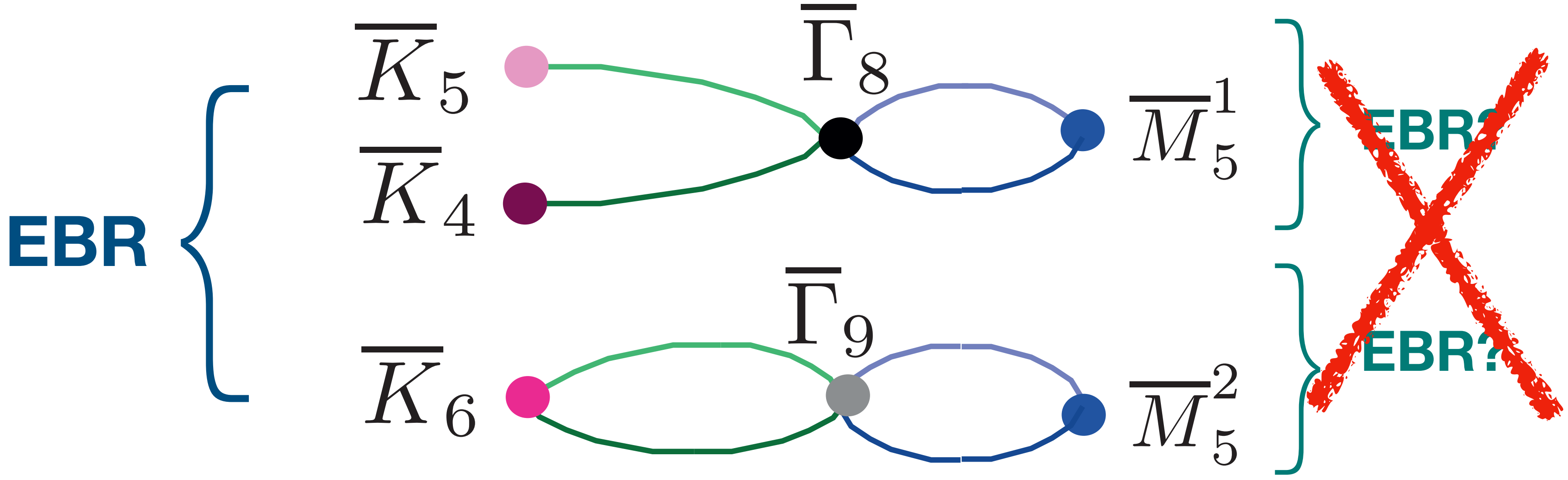
Definition of topological bands

- A group of bands isolated in energy is **topological** if it cannot be smoothly deformed to any atomic limit without either closing the gap or breaking symmetry

Connection to band representations

- Band reps are topologically trivial
- All topologically trivial bands correspond to a band rep

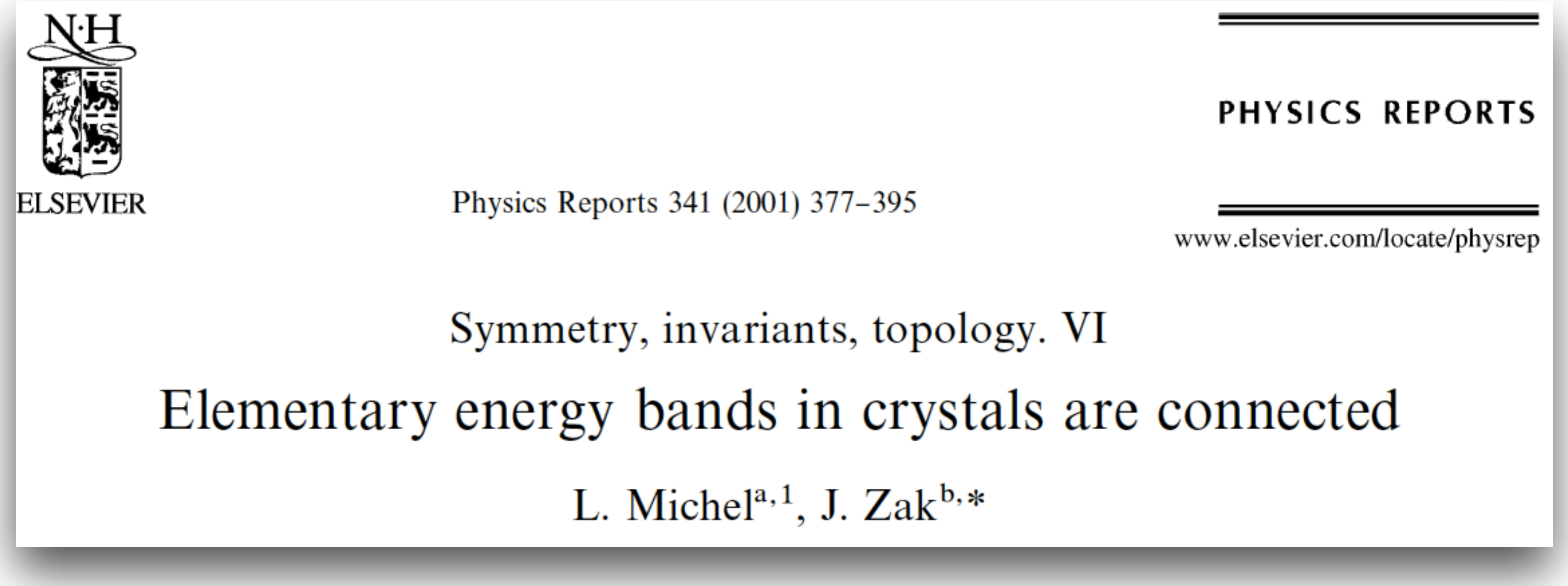
“Disconnected” EBRs are topological



If each group of bands was an EBR, then the sum of both would be composite

⇒ at least one group must be topological

Michel and Zak believed elementary bands could not be gapped



ELSEVIER

PHYSICS REPORTS

Physics Reports 341 (2001) 377–395

www.elsevier.com/locate/physrep

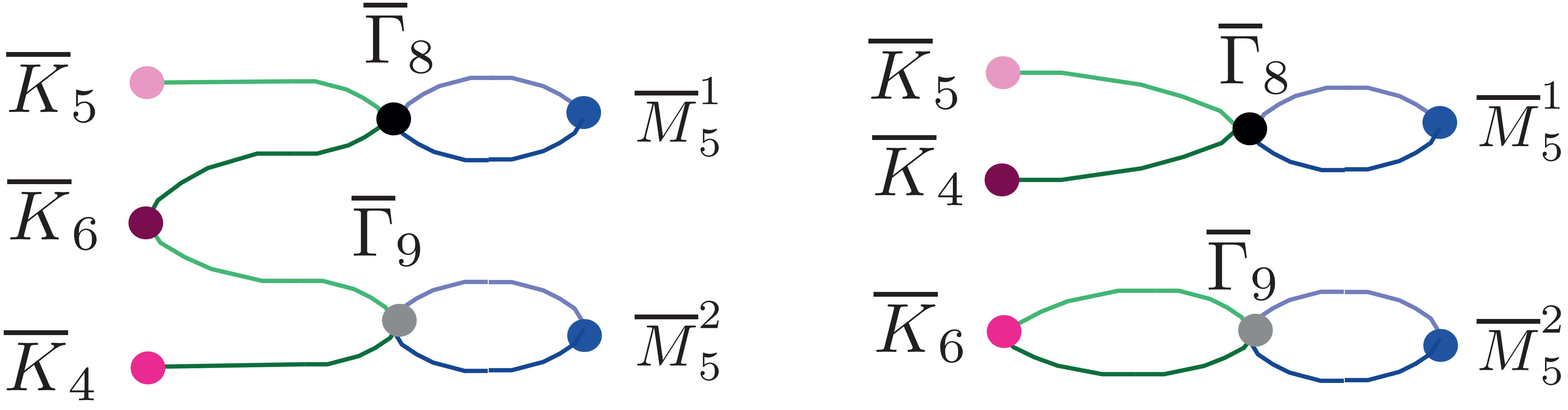
Symmetry, invariants, topology. VI

Elementary energy bands in crystals are connected

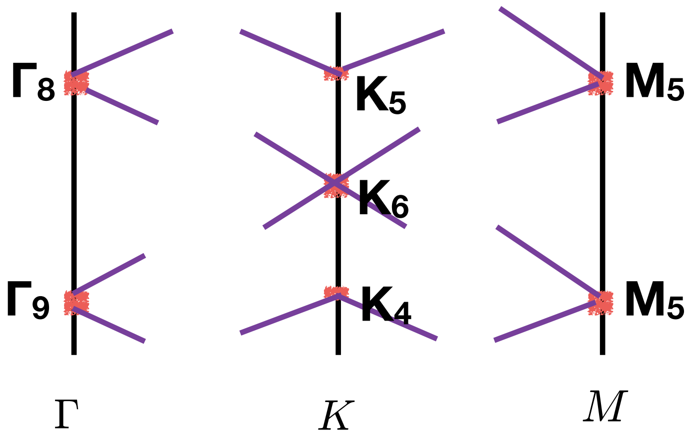
L. Michel[a,1], J. Zak[b,*]

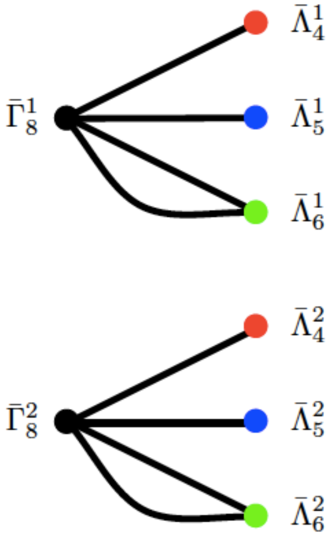
“we present the topologically global concepts necessary for the proof”

Symmetry does not uniquely determine connectivity



Motivated to find connectivity of EBRs: Map to graph theory





Input: irreps at high-symmetry points and lines

Map:
irreps ⇨ graph nodes

Enumerate allowed graphs

For each matrix, null vectors of Laplacian give graph connectivity

Map:
graph connectivity ⇨ band connectivity

Output: distinct band connectivities

$$A_1 = \begin{array}{cc|cccc|cccc|ccc|cccc|cc|c}
\bar{\Gamma}_8 & \bar{\Gamma}_9 & \bar{\Sigma}_3^1 & \bar{\Sigma}_3^2 & \bar{\Sigma}_4^1 & \bar{\Sigma}_4^2 & \bar{\Lambda}_3^1 & \bar{\Lambda}_3^2 & \bar{\Lambda}_4^1 & \bar{\Lambda}_4^2 & \bar{K}_4 & \bar{K}_5 & \bar{K}_6 & \bar{T}_3^1 & \bar{T}_3^2 & \bar{T}_4^1 & \bar{T}_4^2 & \bar{M}_5^1 & \bar{M}_5^2 & \\
0 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \bar{\Gamma}_8 \\
0 & 0 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \bar{\Gamma}_9 \\
\hline
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & \bar{\Sigma}_3^1 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & \bar{\Sigma}_3^2 \\
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & \bar{\Sigma}_4^1 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & \bar{\Sigma}_4^2 \\
\hline
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \bar{\Lambda}_3^1 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & \bar{\Lambda}_3^2 \\
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & \bar{\Lambda}_4^1 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \bar{\Lambda}_4^2 \\
\hline
0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & \bar{K}_4 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & \bar{K}_5 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & \bar{K}_6 \\
\hline
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & \bar{T}_3^1 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & \bar{T}_3^2 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & \bar{T}_4^1 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & \bar{T}_4^2 \\
\hline
0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & \bar{M}_5^1 \\
0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & \bar{M}_5^2
\end{array}$$

Example:

$$\bar{K}_4 \downarrow G_\Lambda = \bar{\Lambda}_3$$

$$\bar{K}_5 \downarrow G_\Lambda = \bar{\Lambda}_4$$

$$\boxed{\bar{K}_6 \downarrow G_\Lambda = \bar{\Lambda}_3 \oplus \bar{\Lambda}_4}$$

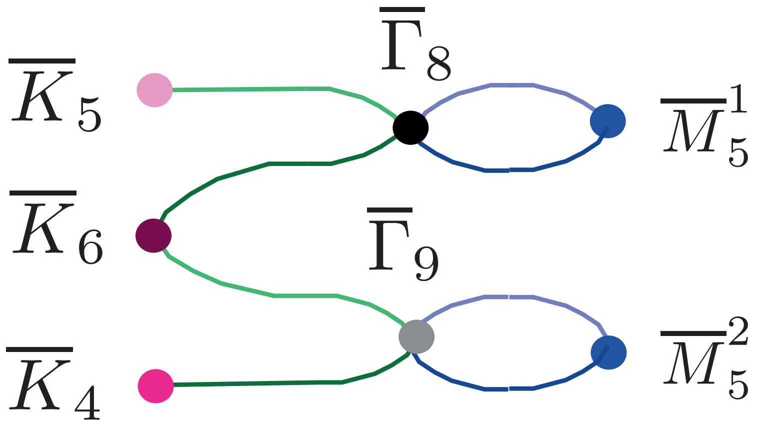
$$\boxed{\bar{\Gamma}_8 \downarrow G_\Lambda = \bar{\Lambda}_3 \oplus \bar{\Lambda}_4}$$

$$\boxed{\bar{\Gamma}_9 \downarrow G_\Lambda = \bar{\Lambda}_3 \oplus \bar{\Lambda}_4}$$

$$\bar{\Gamma}_8 \downarrow G_\Sigma = \bar{\Sigma}_3 \oplus \bar{\Sigma}_4$$

$$\bar{\Gamma}_9 \downarrow G_\Sigma = \bar{\Sigma}_3 \oplus \bar{\Sigma}_4$$

$$\bar{M}_5 \downarrow G_\Sigma = \bar{\Sigma}_3 \oplus \bar{\Sigma}_4$$



← Compatibility relations

$$\begin{array}{cc|cccc|cccc|ccc|cccc|cc|l}
\bar{\Gamma}_8 & \bar{\Gamma}_9 & \bar{\Sigma}_3^1 & \bar{\Sigma}_3^2 & \bar{\Sigma}_4^1 & \bar{\Sigma}_4^2 & \bar{\Lambda}_3^1 & \bar{\Lambda}_3^2 & \bar{\Lambda}_4^1 & \bar{\Lambda}_4^2 & \bar{K}_4 & \bar{K}_5 & \bar{K}_6 & \bar{T}_3^1 & \bar{T}_3^2 & \bar{T}_4^1 & \bar{T}_4^2 & \bar{M}_5^1 & \bar{M}_5^2 & \\
0 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \bar{\Gamma}_8 \\
0 & 0 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \bar{\Gamma}_9 \\
\hline
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & \bar{\Sigma}_3^1 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & \bar{\Sigma}_3^2 \\
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & \bar{\Sigma}_4^1 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & \bar{\Sigma}_4^2 \\
\hline
\boxed{1} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \bar{\Lambda}_3^1 \\
0 & \boxed{1} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \boxed{1} & 0 & 0 & 0 & 0 & 0 & 0 & \bar{\Lambda}_3^2 \\
\boxed{1} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \boxed{1} & 0 & 0 & 0 & 0 & 0 & 0 & \bar{\Lambda}_4^1 \\
0 & \boxed{1} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \bar{\Lambda}_4^2 \\
\hline
0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & \bar{K}_4 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & \bar{K}_5 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & \bar{K}_6 \\
\hline
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & \bar{T}_3^1 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & \bar{T}_3^2 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & \bar{T}_4^1 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & \bar{T}_4^2 \\
\hline
0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & \bar{M}_5^1 \\
0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & \bar{M}_5^2
\end{array}$$

L=D-A has 1 null vector

Example:

$$\boxed{\begin{aligned}\bar{K}_4 \downarrow G_\Lambda &= \bar{\Lambda}_3\\ \bar{K}_5 \downarrow G_\Lambda &= \bar{\Lambda}_4\end{aligned}}$$

$$\boxed{\bar{K}_6 \downarrow G_\Lambda = \bar{\Lambda}_3 \oplus \bar{\Lambda}_4}$$

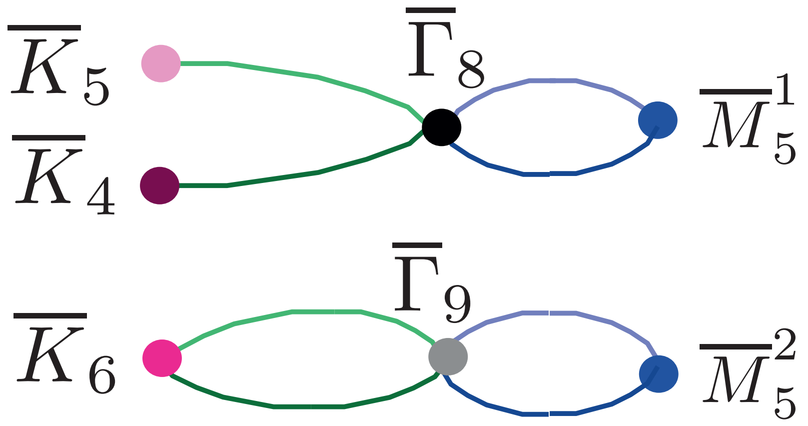
$$\boxed{\bar{\Gamma}_8 \downarrow G_\Lambda = \bar{\Lambda}_3 \oplus \bar{\Lambda}_4}$$

$$\boxed{\bar{\Gamma}_9 \downarrow G_\Lambda = \bar{\Lambda}_3 \oplus \bar{\Lambda}_4}$$

$$\bar{\Gamma}_8 \downarrow G_\Sigma = \bar{\Sigma}_3 \oplus \bar{\Sigma}_4$$

$$\bar{\Gamma}_9 \downarrow G_\Sigma = \bar{\Sigma}_3 \oplus \bar{\Sigma}_4$$

$$\bar{M}_5 \downarrow G_\Sigma = \bar{\Sigma}_3 \oplus \bar{\Sigma}_4$$

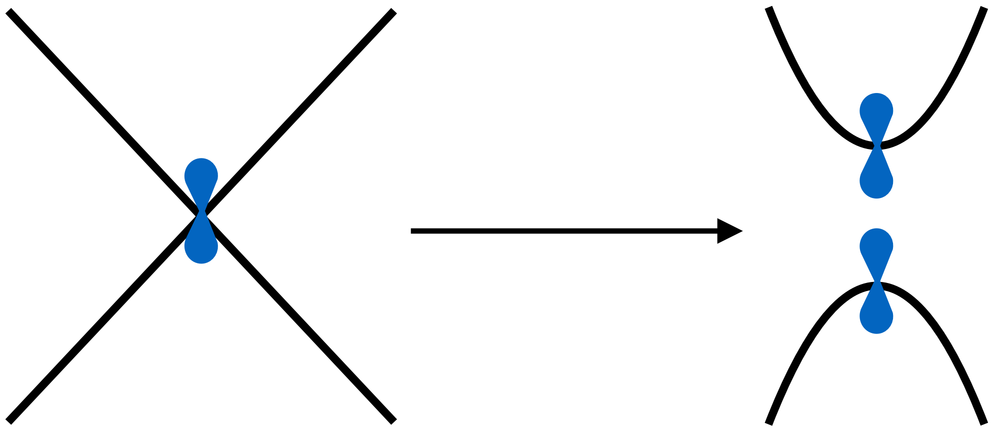


← **Compatibility relations**

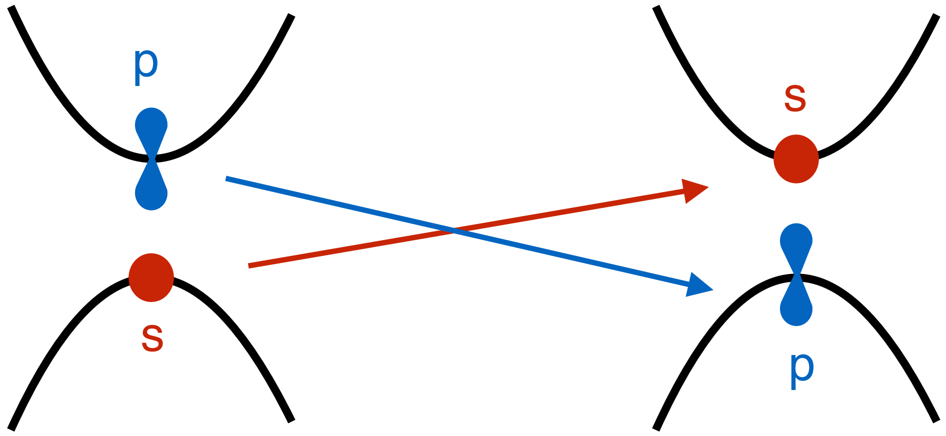
$$\begin{array}{cc|cccc|cccc|ccc|cccc|cc|c}
\bar{\Gamma}_8 & \bar{\Gamma}_9 & \bar{\Sigma}_3^1 & \bar{\Sigma}_3^2 & \bar{\Sigma}_4^1 & \bar{\Sigma}_4^2 & \bar{\Lambda}_3^1 & \bar{\Lambda}_3^2 & \bar{\Lambda}_4^1 & \bar{\Lambda}_4^2 & \bar{K}_4 & \bar{K}_5 & \bar{K}_6 & \bar{T}_3^1 & \bar{T}_3^2 & \bar{T}_4^1 & \bar{T}_4^2 & \bar{M}_5^1 & \bar{M}_5^2 & \\
0 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \bar{\Gamma}_8 \\
0 & 0 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \bar{\Gamma}_9 \\
\hline
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & \bar{\Sigma}_3^1 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & \bar{\Sigma}_3^2 \\
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & \bar{\Sigma}_4^1 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & \bar{\Sigma}_4^2 \\
\hline
\boxed{1} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \boxed{1} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \bar{\Lambda}_3^1 \\
0 & \boxed{1} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \boxed{1} & 0 & 0 & 0 & 0 & 0 & 0 & \bar{\Lambda}_3^2 \\
\boxed{1} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \boxed{1} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \bar{\Lambda}_4^1 \\
0 & \boxed{1} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \boxed{1} & 0 & 0 & 0 & 0 & 0 & 0 & \bar{\Lambda}_4^2 \\
\hline
0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & \bar{K}_4 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & \bar{K}_5 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & \bar{K}_6 \\
\hline
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & \bar{T}_3^1 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & \bar{T}_3^2 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & \bar{T}_4^1 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & \bar{T}_4^2 \\
\hline
0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & \bar{M}_5^1 \\
0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & \bar{M}_5^2
\end{array}$$

L=D-A has 2 null vectors

Routes to topological bands:



Disconnected elementary
band representation
(e.g., graphene)



Multiple EBRs + band inversion

(e.g., HgTe)

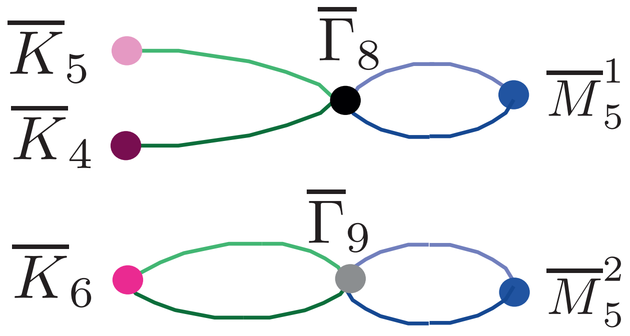
Part 3: How to identify (non) - EBRs and applications

Tool: vector of irreps at high-symmetry points

1. List all maximal high-symmetry points and all possible irreps

Ex: $(\bar{\Gamma}_7, \bar{\Gamma}_8, \bar{\Gamma}_9, \bar{K}_4, \bar{K}_5, \bar{K}_6, \bar{M}_5)$

2. List the number of times each irrep appears



Ex conduction: $(0, 1, 0, 1, 1, 0, 1)$

valence: $(0, 0, 1, 0, 0, 1, 1)$

For EBRs, these vectors can be obtained from BANDREP

3. For topologically trivial bands, the vector must be a sum of vectors corresponding EBRs

Case 1: irreps at all high-symmetry points not equal to a sum of EBRs

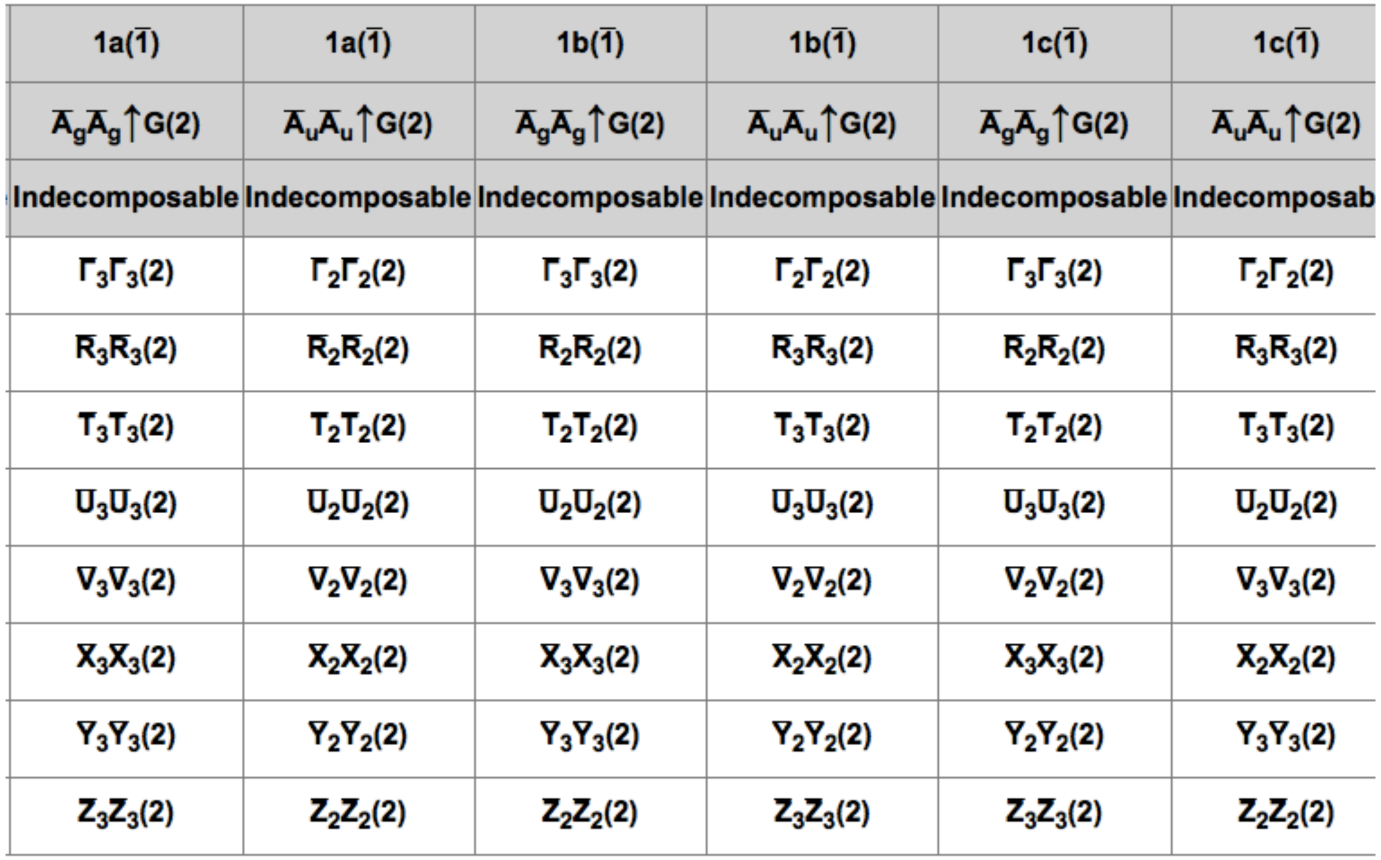
Cannot be a band rep ⇒ must be topological

Example: Fu-Kane inversion eigenvalue index

PRB 76, 045302 (2007)

$$(-1)^{\nu} = \prod_i \delta_i$$

Elementary band-representations with time-reversal symmetry of the Double Space Group *P*$\bar{1}$ (No. 2)



1a($\bar{1}$)	1a($\bar{1}$)	1b($\bar{1}$)	1b($\bar{1}$)	1c($\bar{1}$)	1c($\bar{1}$)
$\bar{A}_g\bar{A}_g\uparrow G(2)$	$\bar{A}_u\bar{A}_u\uparrow G(2)$	$\bar{A}_g\bar{A}_g\uparrow G(2)$	$\bar{A}_u\bar{A}_u\uparrow G(2)$	$\bar{A}_g\bar{A}_g\uparrow G(2)$	$\bar{A}_u\bar{A}_u\uparrow G(2)$
Indecomposable	Indecomposable	Indecomposable	Indecomposable	Indecomposable	Indecomposab
$\bar{\Gamma}_3\bar{\Gamma}_3(2)$	$\bar{\Gamma}_2\bar{\Gamma}_2(2)$	$\bar{\Gamma}_3\bar{\Gamma}_3(2)$	$\bar{\Gamma}_2\bar{\Gamma}_2(2)$	$\bar{\Gamma}_3\bar{\Gamma}_3(2)$	$\bar{\Gamma}_2\bar{\Gamma}_2(2)$
$\bar{R}_3\bar{R}_3(2)$	$\bar{R}_2\bar{R}_2(2)$	$\bar{R}_2\bar{R}_2(2)$	$\bar{R}_3\bar{R}_3(2)$	$\bar{R}_2\bar{R}_2(2)$	$\bar{R}_3\bar{R}_3(2)$
$\bar{T}_3\bar{T}_3(2)$	$\bar{T}_2\bar{T}_2(2)$	$\bar{T}_2\bar{T}_2(2)$	$\bar{T}_3\bar{T}_3(2)$	$\bar{T}_2\bar{T}_2(2)$	$\bar{T}_3\bar{T}_3(2)$
$\bar{U}_3\bar{U}_3(2)$	$\bar{U}_2\bar{U}_2(2)$	$\bar{U}_2\bar{U}_2(2)$	$\bar{U}_3\bar{U}_3(2)$	$\bar{U}_3\bar{U}_3(2)$	$\bar{U}_2\bar{U}_2(2)$
$\bar{V}_3\bar{V}_3(2)$	$\bar{V}_2\bar{V}_2(2)$	$\bar{V}_3\bar{V}_3(2)$	$\bar{V}_2\bar{V}_2(2)$	$\bar{V}_2\bar{V}_2(2)$	$\bar{V}_3\bar{V}_3(2)$
$\bar{X}_3\bar{X}_3(2)$	$\bar{X}_2\bar{X}_2(2)$	$\bar{X}_3\bar{X}_3(2)$	$\bar{X}_2\bar{X}_2(2)$	$\bar{X}_3\bar{X}_3(2)$	$\bar{X}_2\bar{X}_2(2)$
$\bar{Y}_3\bar{Y}_3(2)$	$\bar{Y}_2\bar{Y}_2(2)$	$\bar{Y}_3\bar{Y}_3(2)$	$\bar{Y}_2\bar{Y}_2(2)$	$\bar{Y}_2\bar{Y}_2(2)$	$\bar{Y}_3\bar{Y}_3(2)$
$\bar{Z}_3\bar{Z}_3(2)$	$\bar{Z}_2\bar{Z}_2(2)$	$\bar{Z}_2\bar{Z}_2(2)$	$\bar{Z}_3\bar{Z}_3(2)$	$\bar{Z}_3\bar{Z}_3(2)$	$\bar{Z}_2\bar{Z}_2(2)$

...

Exercise: check for all EBRs in $P\bar{1}, \nu = 0$

Case 2: irreps at all high-symmetry points equal to a sum of EBRs

Could be trivial or topological

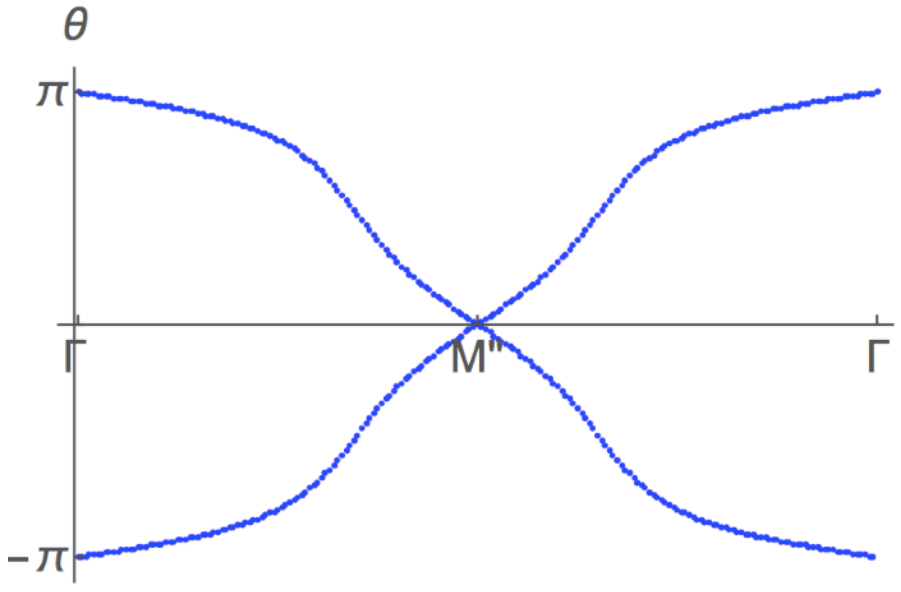
Ex: space group P1

What to do???

Topological bands not deformable to EBRs

For each sum of EBRs with matching irreps, check whether smooth deformation is possible

If topological, will differ by another quantized invariant (Berry phase, Wilson loop, …)

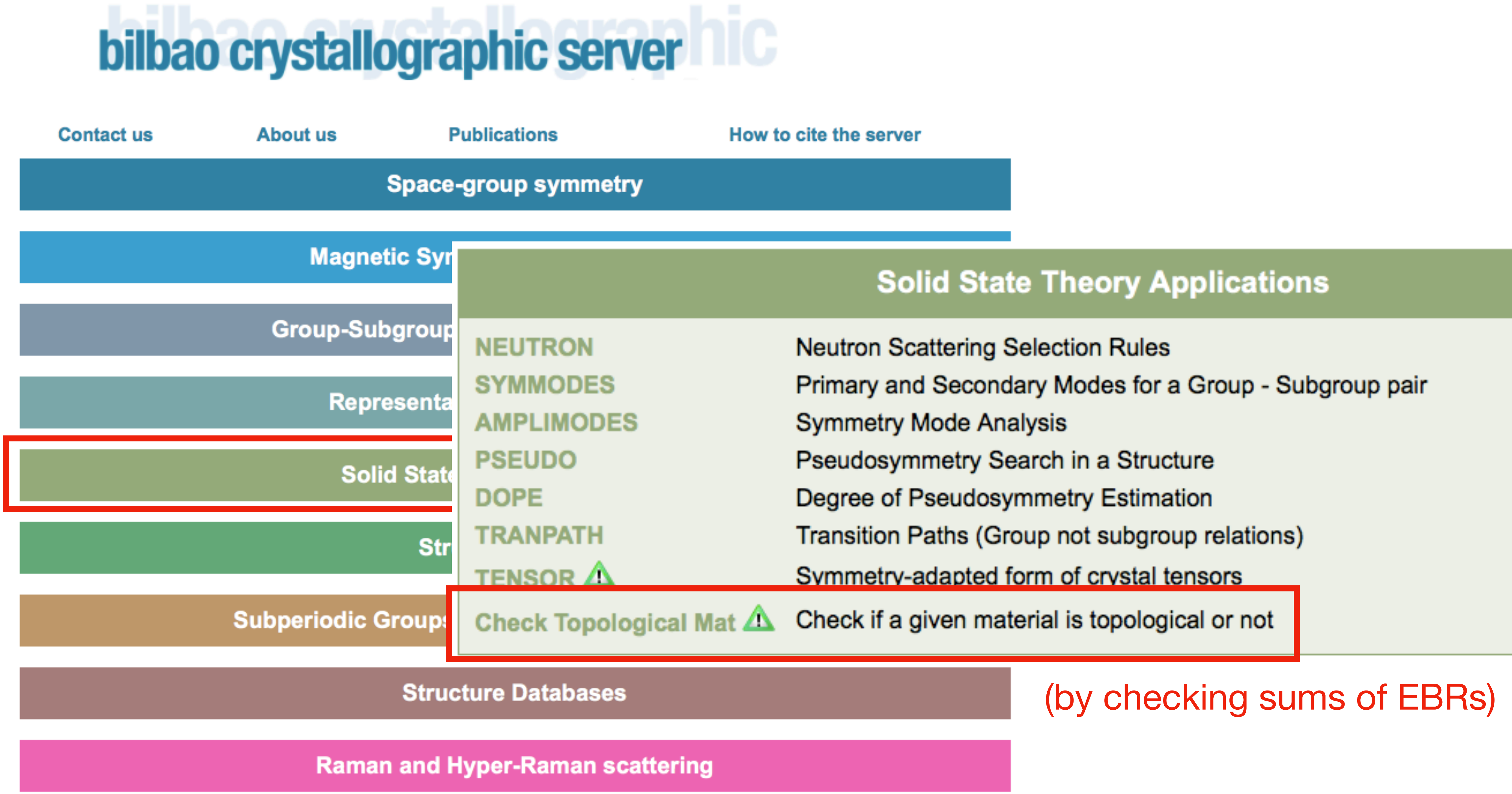


Conclude: symmetry eigenvalues are not the whole story…
… but since most crystals have symmetry, they are useful in many cases

Application: check topo mat

Ref: "All the (high-quality) topological materials in the world,"
Vergniory, Elcoro, Felser, Bernevig, Wang, ArXiv: 1807.10271

http://www.cryst.ehu.es/cgi-bin/cryst/programs/topological.pl



bilbao crystallographic server

Contact us About us Publications How to cite the server

Space-group symmetry

Magnetic Sy

Group-Subgroup

Representa

Solid Stat

Str

Subperiodic Groups

Structure Databases

Raman and Hyper-Raman scattering

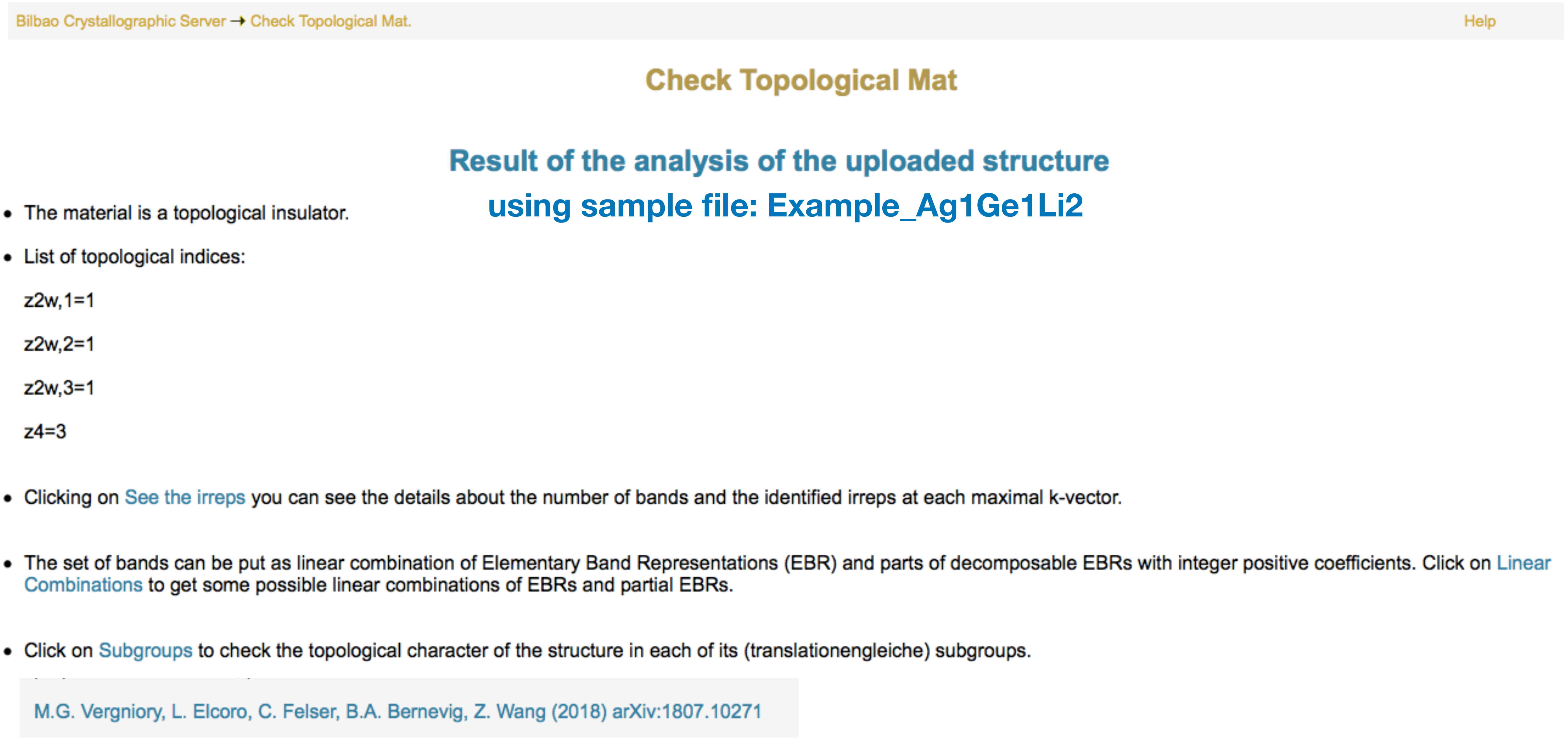
Solid State Theory Applications

NEUTRON	Neutron Scattering Selection Rules
SYMMODES	Primary and Secondary Modes for a Group - Subgroup pair
AMPLIMODES	Symmetry Mode Analysis
PSEUDO	Pseudosymmetry Search in a Structure
DOPE	Degree of Pseudosymmetry Estimation
TRANPATH	Transition Paths (Group not subgroup relations)
TENSOR ⚠	Symmetry-adapted form of crystal tensors
Check Topological Mat ⚠	Check if a given material is topological or not

(by checking sums of EBRs)

Application: check topo mat

Ref: "All the (high-quality) topological materials in the world,"
Vergniory, Elcoro, Felser, Bernevig, Wang, ArXiv: 1807.10271



Check Topological Mat

Result of the analysis of the uploaded structure

using sample file: Example_Ag1Ge1Li2

- The material is a topological insulator.
- List of topological indices:

  z2w,1=1

  z2w,2=1

  z2w,3=1

  z4=3

- Clicking on See the irreps you can see the details about the number of bands and the identified irreps at each maximal k-vector.
- The set of bands can be put as linear combination of Elementary Band Representations (EBR) and parts of decomposable EBRs with integer positive coefficients. Click on Linear Combinations to get some possible linear combinations of EBRs and partial EBRs.
- Click on Subgroups to check the topological character of the structure in each of its (translationengleiche) subgroups.

M.G. Vergniory, L. Elcoro, C. Felser, B.A. Bernevig, Z. Wang (2018) arXiv:1807.10271

Authors have carried out this procedure for all high-quality materials in the ICSD

Application: Materiae

Ref: “Catalogue of electronic topological materials,” Zhang, et al
ArXiv: 1807.08756, (Chen Fang’s group).

http://materiae.iphy.ac.cn/

✱ Record for SnTe

Non-SOC Topological Info

Topological Class	High symmetry line semi-metal
High Symmetry Lines	M-X, X-R

SOC Topological Info

Topological class	Topological insulator
Symmetry-based Indicator	1, 7
Indicator Group	Z4, Z8

Symmetry-based indicators of topology

Ref: “Symmetry-based indicators of band topology in the 230 space groups,” Po, Vishwanath, Watanabe, ArXiv: 1703.00911, Nature Comm. 8, 50 (2017)

Recall: each EBR is assigned a vector of irreps at high-symmetry points:

$$\mathbf{v}_{(\rho,w)} = (n_{\mathbf{k}_1,1}, n_{\mathbf{k}_1,2}, n_{\mathbf{k}_2,1}, \ldots..)$$

irrep   Wyckoff position

Band reps are sums of EBRs:

$$S_{\mathrm{BR}} = \sum_{(\rho,w)\in \mathrm{EBR}} c_{(\rho,w)} \mathbf{v}_{(\rho,w)}$$

integer coefficient   EBR vector

Solutions to compatibility relations: $S_{CR} = \{\mathbf{w} | \mathbf{w} \text{ satisfies compatibility}\}$

⇒ Elements in the set S_{CR}/S_{BR} necessarily describe topological bands

but some topological bands are marked as trivial

Compare EBRs and symmetry indicators

	EBRs	**Symmetry indicators**
Predictive power	Yes	No
Provide Z_n index	No	Yes
Topo. bands can be classified as trivial	No*	Yes

*caveat: not always easy to answer this question

When are topological bands missed by symmetry indicators?

$$S_{\mathrm{BR}} = \sum_{(\rho,w)\in\mathrm{EBR}} c_{(\rho,w)}\mathbf{v}_{(\rho,w)} \qquad S_{CR} = \{\mathbf{w}|\mathbf{w} \text{ satisfies compatibility}\}$$

Case 1: not enough symmetry

Recall example of SG P1: this case is also difficult to detect from EBRs

Case 2: negative coefficients $c_{(\rho,w)}$

This case is detectable from EBRs (now included on BCS in check topo mat)

“Fragile topology”

What does this mean for gapped EBRs?

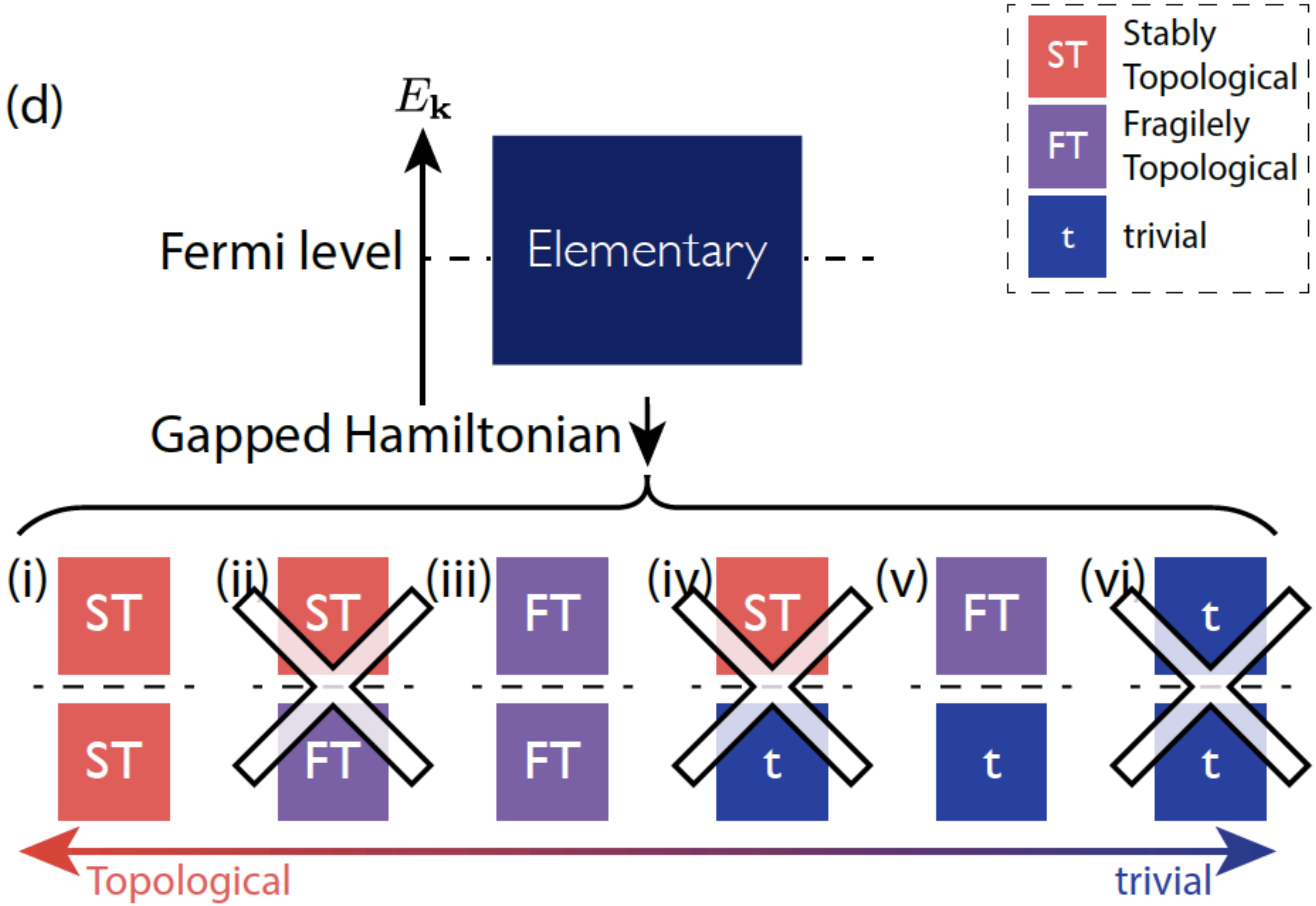


Figure: Po, Watanabe and Vishwanath, ArXiv: 1709.06551

Exercises

Fu-Kane formula. Recall the Fu-Kane formula: a group of bands is a topological insulator protected by time-reversal symmetry if the product of inversion eigenvalues (one from each Kramers pair) is equal to -1. Using the table of inversion eigenvalues in P-1, prove that all band reps in the space group have a trivial Fu-Kane index. (Note: this makes sense because all band reps are topologically trivial.)

Symmetry indicator with inversion symmetry. In P-1, the vector of symmetry eigenvalues for a group of bands is given by:
($n_{\Gamma+}$, $n_{\Gamma-}$, n_{R+}, n_{R-}, n_{T+}, n_{T-}, n_{U+}, n_{U-}, n_{V+}, n_{V-}, n_{X+}, n_{X-}, n_{Y+}, n_{Y-}, n_{Z+}, n_{Z-},),
where $n_{\mathbf{k}+}$, $n_{\mathbf{k}-}$, are the number of bands at **k** with inversion eigenvalue + or -. There are no constraints from the compatibility relations, but for a group of n bands, it must be that $n_{\mathbf{k}+} + n_{\mathbf{k}-} = n$ for all **k.**

a) Write the vector for each EBR.

b) Prove that $\Sigma_{\mathbf{k}} (n_{\mathbf{k}+} - n_{\mathbf{k}-})$ is a multiple of 8 for an EBR.

c) Prove that in general, $\Sigma_{\mathbf{k}} (n_{\mathbf{k}+} - n_{\mathbf{k}-})$ is even, whether or not the bands are an EBR.

c) Bonus: when the bands obey time-reversal symmetry, $n_{\mathbf{k}+} \rightarrow 2n_{\mathbf{k}+}$, $n_{\mathbf{k}-} \rightarrow 2n_{\mathbf{k}-}$. Prove that there is a Z_4 index which is zero for EBRs and non-zero otherwise.

Graph theory exercise

Given a graph with labelled (numbered) nodes, the degree matrix, D, has diagonal entries indicating the number of lines coming out of each node. The adjacency matrix, A, has $A_{ij} = A_{ji} = n$ if there are n lines connecting node i and node j. Each zero eigenvector of the Laplacian matrix, L = D - A, indicates a connected component of the graph by its non-zero entries. See below for an example (from Wikipedia).

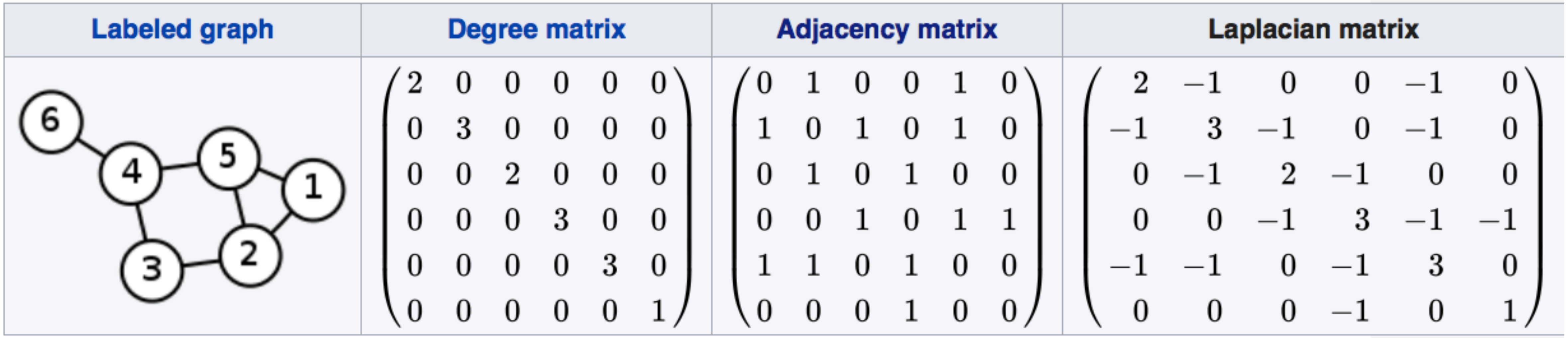
a) Find the zero eigenvector of the Laplacian matrix below.

b) Prove that the diagonal entries of L are always non-negative, while the off-diagonal entries are always non-positive.

c) Prove that the sum of the entries in each row/column of L is zero.

d) Prove that the vector (1, 1, …., 1) is always a zero eigenvector of L, as long as each line connects to one node at either end; lines connecting a node to itself are allowed.

e) Prove that a disconnected component of the graph always contributes a zero eigenvector to L.



Labeled graph	**Degree matrix**	**Adjacency matrix**	**Laplacian matrix**
	$\begin{pmatrix} 2&0&0&0&0&0\\ 0&3&0&0&0&0\\ 0&0&2&0&0&0\\ 0&0&0&3&0&0\\ 0&0&0&0&3&0\\ 0&0&0&0&0&1 \end{pmatrix}$	$\begin{pmatrix} 0&1&0&0&1&0\\ 1&0&1&0&1&0\\ 0&1&0&1&0&0\\ 0&0&1&0&1&1\\ 1&1&0&1&0&0\\ 0&0&0&1&0&0 \end{pmatrix}$	$\begin{pmatrix} 2&-1&0&0&-1&0\\ -1&3&-1&0&-1&0\\ 0&-1&2&-1&0&0\\ 0&0&-1&3&-1&-1\\ -1&-1&0&-1&3&0\\ 0&0&0&-1&0&1 \end{pmatrix}$