Complete Theory of Symmetry-based Indicators of Band Topology

Haruki Watanabe
University of Tokyo

based on
H.C.Po, A. Vishwanath, HW, arXiv:1703.0091

Fu-Kane formula for Inversion-symmetric TI

- Strong index

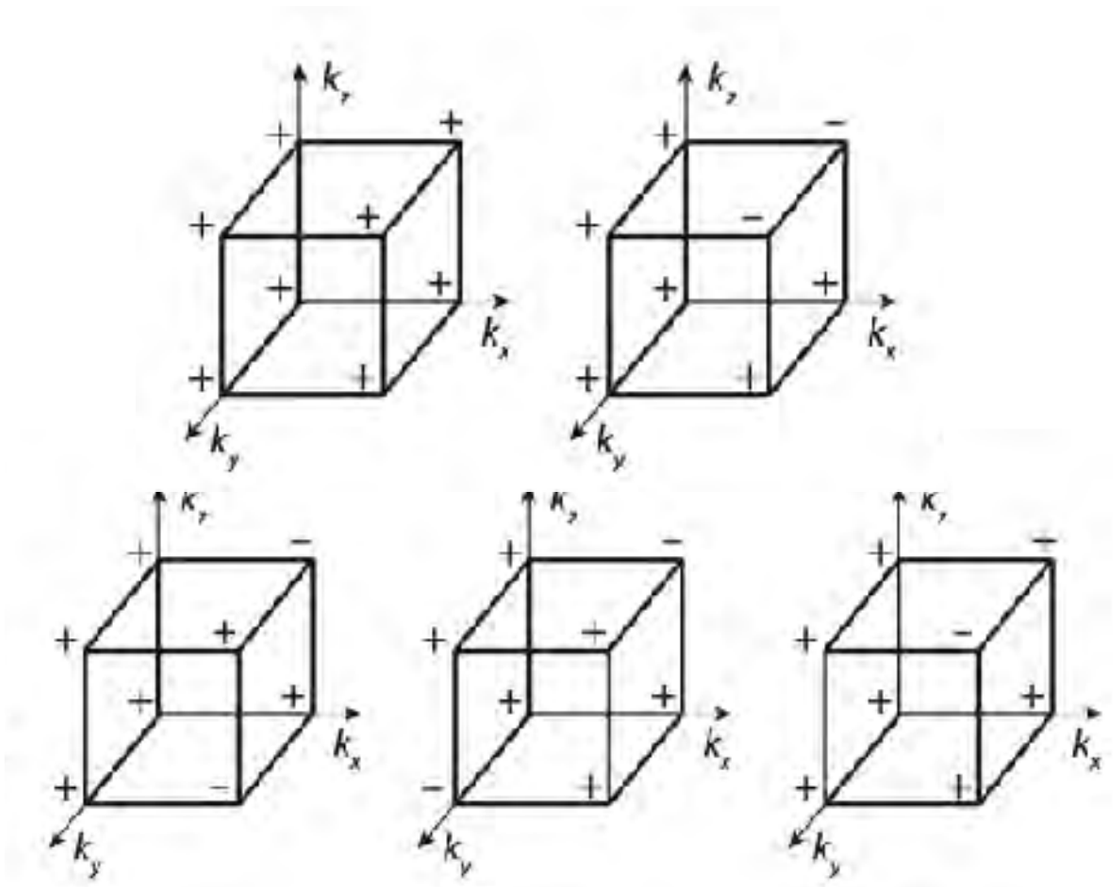
$\nu_0 = \prod_{i,\, j\, ,k\, = 0,\, \pi} \xi_{(i,\, j,\, k)}$

- Weak indices

$\nu_1 = \prod_{j,\, k\, = 0,\, \pi} \xi_{(\pi,\, j,\, k)}$

$\nu_2 = \prod_{i,\, k\, = 0,\, \pi} \xi_{(i,\, \pi,\, k)}$

$\nu_3 = \prod_{i,\, j\, = 0,\, \pi} \xi_{(i,\, j,\, \pi)}$



irreps at high-sym momenta

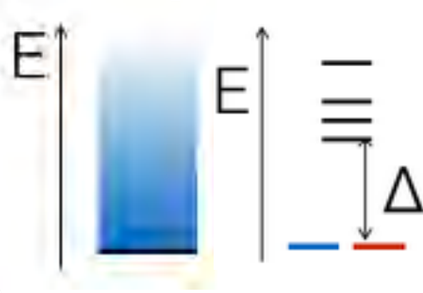
Combination of ~~inversion eigenvalues~~ *indicates*

band insulator is ~~TI protected by TR~~.

nontrivial (not adiabatically connected to the atomic limit)

(Improvement of Lieb-Schultz-Mattis theorem)

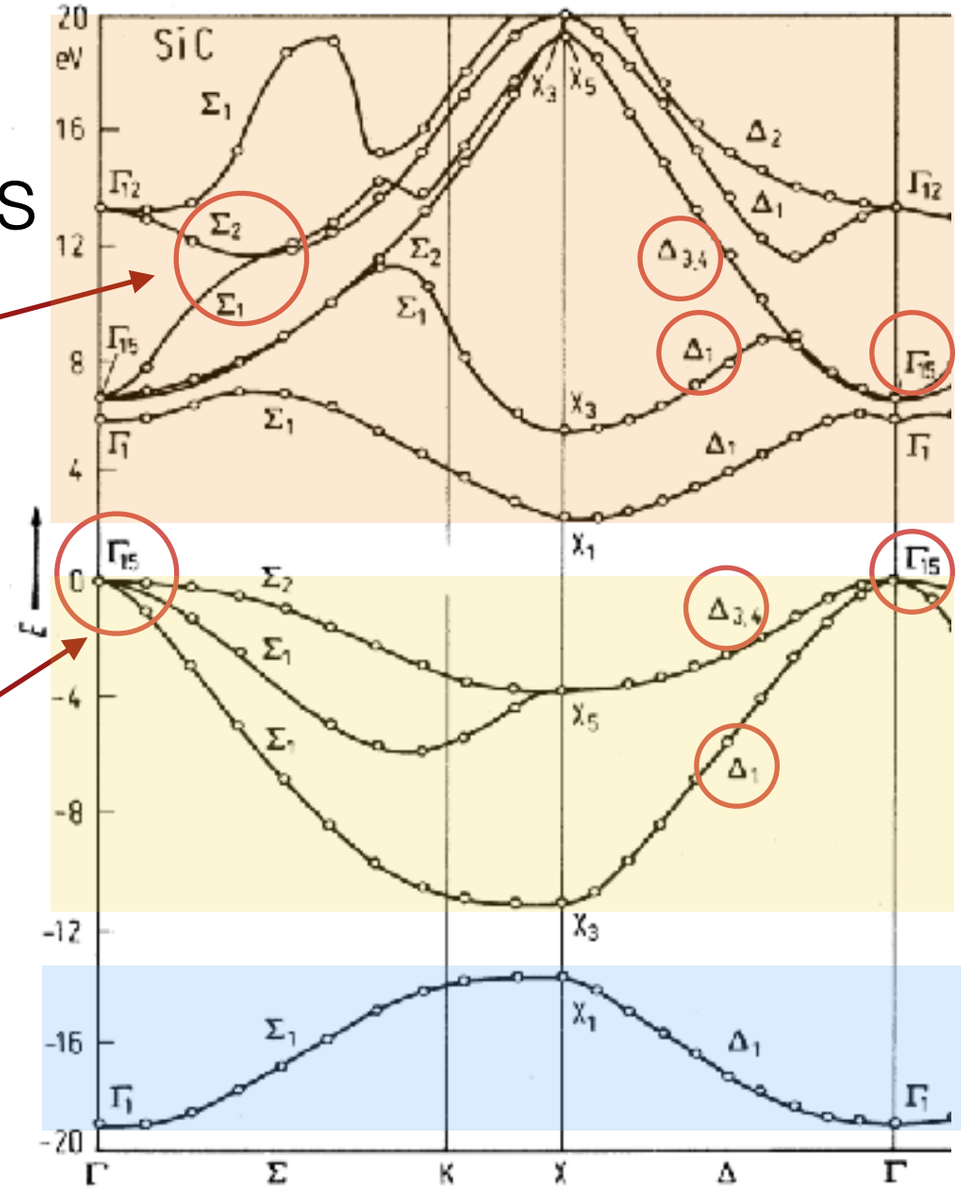
- Assume U(1) symmetry + lattice translations.
- Depending on filling ν, *"unique gapped GS"* is prohibited.



typical band structure…

Bands can cross only when different irreps

Dimensions of the irreps → degeneracy

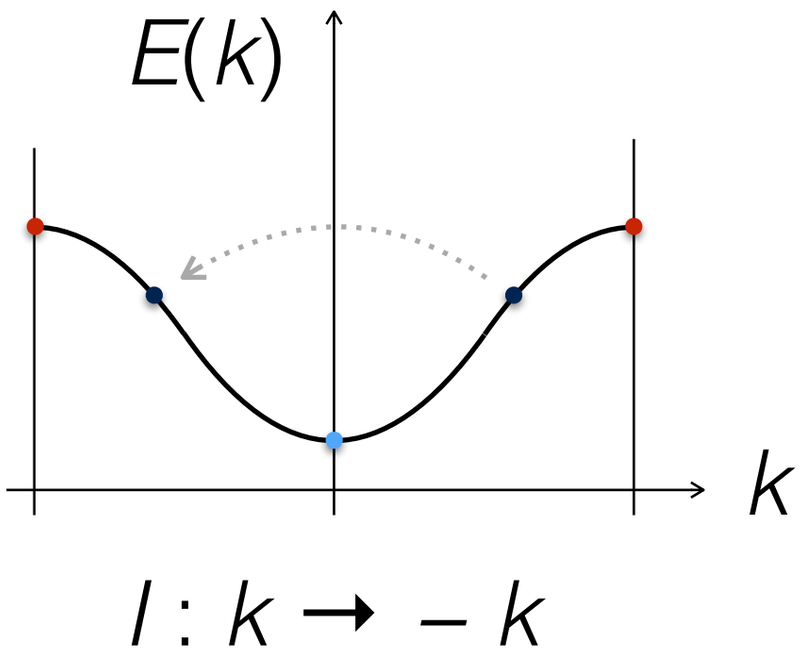


[Hemstreet & Fong (1974)]

Relation among irreps upon symmetry lowering

Topological properties
(i) Assume band gap at high sym momenta
(ii) Forget energetics within a set of bands

Example:
Inversion-symmetric 1D chain



- Two invariant momenta
  $k = 0, \pi$

  → *High-symmetry momenta*
  Little group of k, G_k

- Inversion eigenvalues
  $I = \pm 1$

  → *Irreducible representation of G_k*

Example: Inversion-symmetric 1D chain

$n_{\boldsymbol{k}}^{\alpha}$: the number of times an irrep $u_{\boldsymbol{k}}^{\alpha}$ appears in BS

$$\boldsymbol{b} = (n_{0}^{+},\ n_{0}^{-},\ n_{\pi}^{+},\ n_{\pi}^{-})$$

	$k = 0$	$k = \pi$
I	+1	+1
	-1	-1
	+1	-1
	-1	+1

$$\boldsymbol{b}_1 = (\ 1\ ,\ 0\ ,\ 1\ ,\ 0\ )$$

$$\boldsymbol{b}_2 = (\ 0\ ,\ 1\ ,\ 0\ ,\ 1\ )$$

$$\boldsymbol{b}_3 = (\ 1\ ,\ 0\ ,\ 0\ ,\ 1\ )$$

$$\boldsymbol{b}_4 = (\ 0\ ,\ 1\ ,\ 1\ ,\ 0\ )$$

$$\boldsymbol{b}_1 + \boldsymbol{b}_2 = \boldsymbol{b}_3 + \boldsymbol{b}_4$$

Four possible combinations

Only three are independent

Example: Inversion-symmetric 1D chain

$$\boldsymbol{b} = (n_{0}^{+},\ n_{0}^{-},\ n_{\pi}^{+},\ n_{\pi}^{-})$$

Relation among $n_{\boldsymbol{k}}^{\alpha}$'s

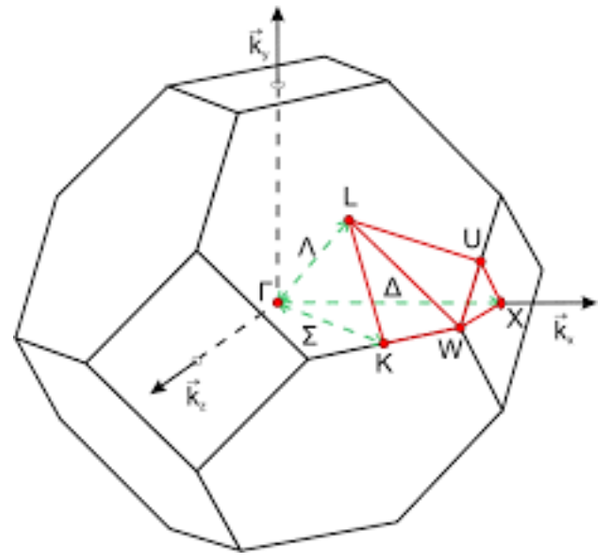
$$n_{0}^{+} + n_{0}^{-} = n_{\pi}^{+} + n_{\pi}^{-} = \mathrm{v}\ (= \#\ \text{of bands})$$

$$\boldsymbol{b} = n_{0}^{+}\,(1, -1, 0, 0) + n_{\pi}^{+}\,(0, 0, 1, -1) + v\ (0, 1, 0, 1)$$

$$\rightarrow \{\mathrm{BS}\} \equiv \text{set of valid } \boldsymbol{b}\text{'s} = Z^{3}$$

Note: we extended possible values of n to *all integers*
(Classification stable against *subtracting* bands)

Group structure of Band structure



- ***k*** : a high-sym mometum.

Collect all different *types* of ***k***

- $G_{\boldsymbol{k}}$: the little group of ***k***. i.e., { g in G | $g\boldsymbol{k} = \boldsymbol{k} + \boldsymbol{G}$ }

- $u_{\boldsymbol{k}}^{\alpha}$ (α = 1, 2, …): irreducible representation of $G_{\boldsymbol{k}}$

single rep for spinless electrons

double reps for spinful electrons

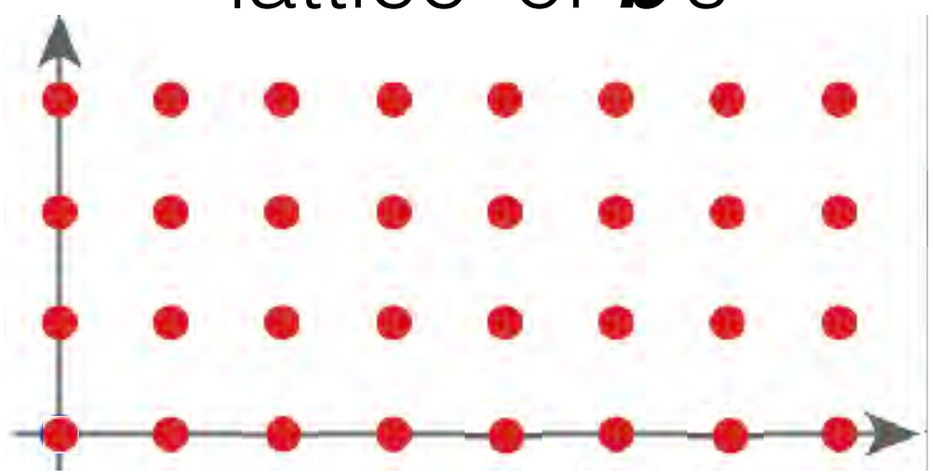
Group structure of Band structure

- $n_{\boldsymbol{k}}^{\alpha}$: the number of times $u_{\boldsymbol{k}}^{\alpha}$ appears in band structure
- $\boldsymbol{b} = (n_{\boldsymbol{k}_1}{}^1, n_{\boldsymbol{k}_1}{}^2, \ldots n_{\boldsymbol{k}_2}{}^1, n_{\boldsymbol{k}_2}{}^2, \ldots)$
- Compatibility relations (+ TR sym) among $\{n_{\boldsymbol{k}}^{\alpha}\}$
- The set of valid $\boldsymbol{b}$'s : $\{\mathrm{BS}\} = Z^{d_{\mathrm{BS}}}$

$$\sum_i m_i \boldsymbol{b}_i \in \{\mathrm{BS}\}$$

Kruthoff *et al.* arXiv:1703.09706
- spinless electrons in 2D
- K-theory calculation

'lattice' of $\boldsymbol{b}$'s



Bloch vs Wannier

H. C. Po, HW, M.P. Zaletel & A. Vishwanath,
Science Adv. 2(4), e1501782 (2016)

- Momentum space picture

  Representations of $G_{\boldsymbol{k}}$

  $\boldsymbol{b} = (n_{\boldsymbol{k}1}{}^1, n_{\boldsymbol{k}1}{}^2, \ldots n_{\boldsymbol{k}2}{}^1, n_{\boldsymbol{k}2}{}^2, \ldots)$

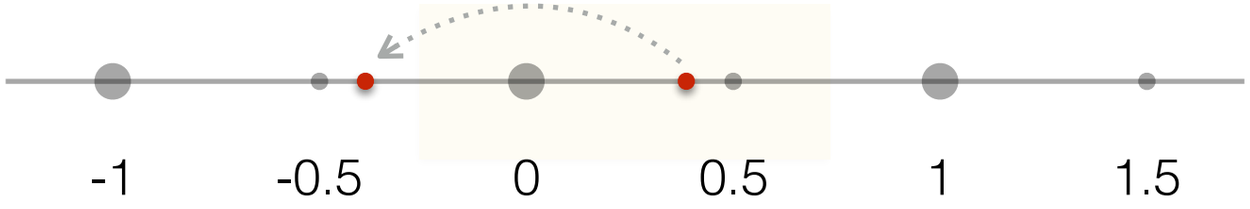
- Real space picture

Atomic Insulators (hopping → 0 limit. Product state)	=	Wannier orbitals (symmetric, exponentially-localized)

Defines the trivial class of {BS}

Example:
Inversion-symmetric 1D chain

- Two symmetric positions (in UC)
  $x = 0, 1/2$



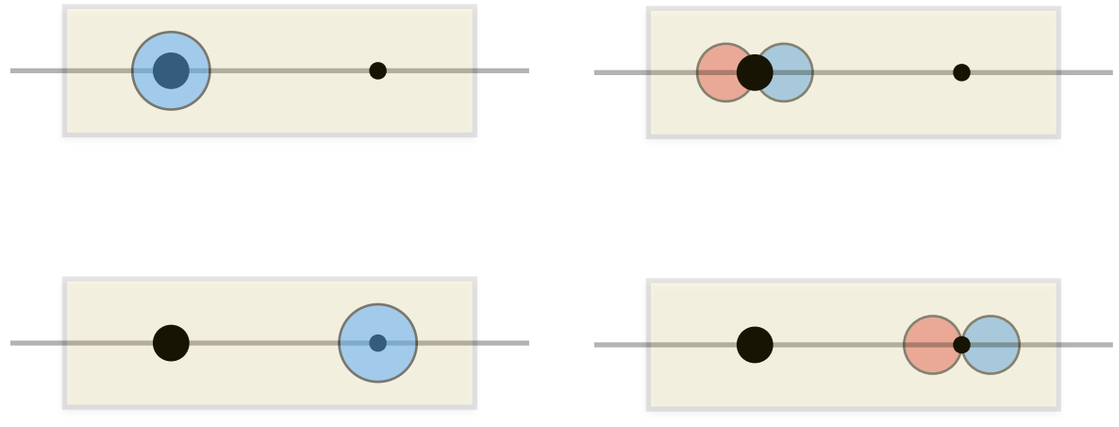
→ *Special position (Wyckoff position)*

Little group of x, G_x

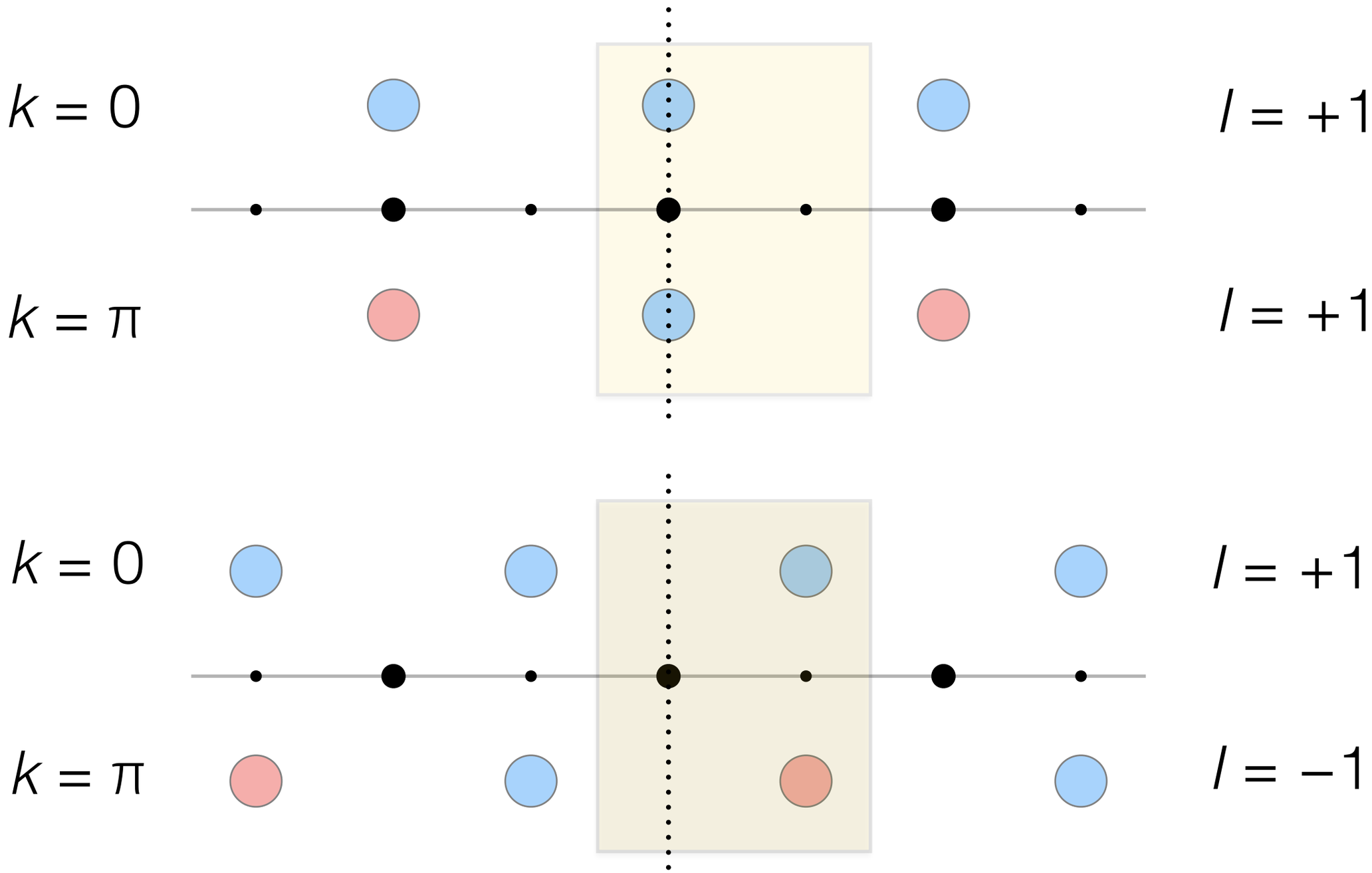
- Parity even/odd orbital

$I = +1$ $I = -1$

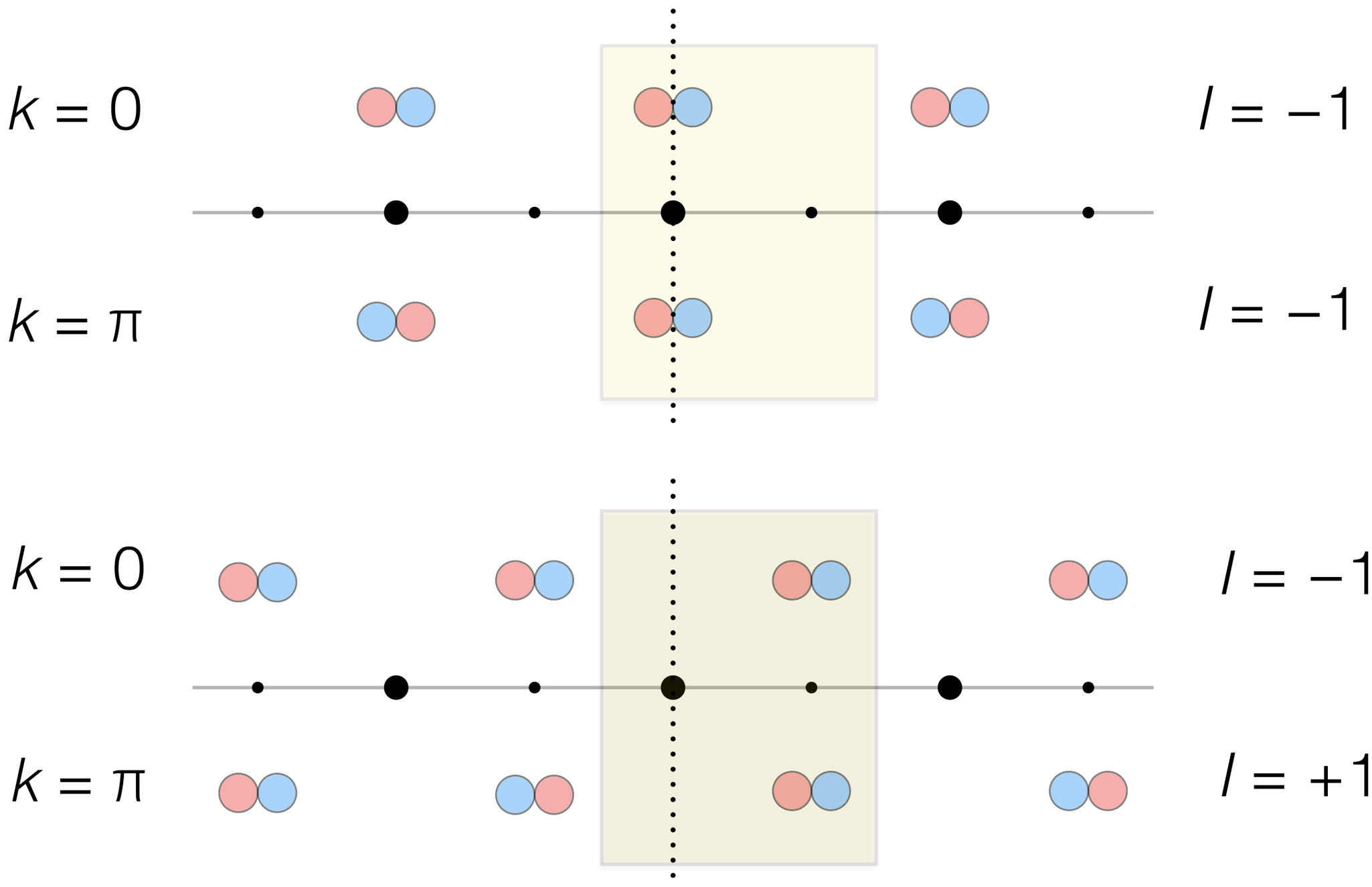
→ *Irreducible representation of G_x*



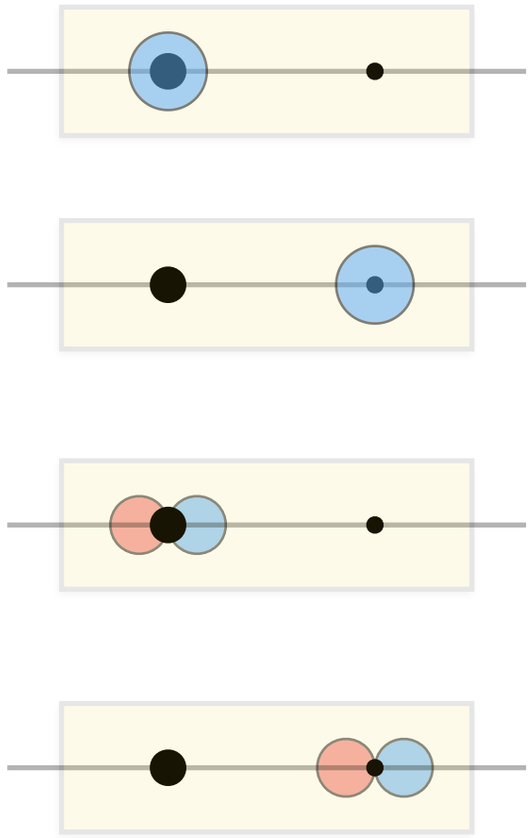
Example:
Inversion-symmetric 1D chain



Example:
Inversion-symmetric 1D chain



Example:
Inversion-symmetric 1D chain



$\boldsymbol{a}_1 = (\ 1\ ,\ 0\ ,\ 1\ ,\ 0\ )$

$\boldsymbol{a}_3 = (\ 1\ ,\ 0\ ,\ 0\ ,\ 1\ )$

$\boldsymbol{a}_2 = (\ 0\ ,\ 1\ ,\ 0\ ,\ 1\ )$

$\boldsymbol{a}_4 = (\ 0\ ,\ 1\ ,\ 1\ ,\ 0\ )$

$\boldsymbol{a}_1 + \boldsymbol{a}_2 = \boldsymbol{a}_3 + \boldsymbol{a}_4$

Set of all $\boldsymbol{b}$ corresponding to AI: $\{AI\} = Z^3$

In this example, {BS} = {AI} (but not necessarily in general)

Listing up all atomic insulators

- $\boldsymbol{x}$: chosen from a special Wyckoff position.
- $G_{\boldsymbol{x}}$: the little group of $\boldsymbol{x}$. i.e., { g in G | $g\boldsymbol{x} = \boldsymbol{x}$ }
- $u_{\boldsymbol{x}}{}^{\alpha}$ (α = 1, 2, …): irreducible representation of $G_{\boldsymbol{x}}$
- The combination ($\boldsymbol{x}$, $u_{\boldsymbol{x}}{}^{\alpha}$) determines AI and its $\boldsymbol{b}$
- Set of all $\boldsymbol{a}$'s corresponding to AI: $\{\mathrm{AI}\} = Z^{d_{\mathrm{AI}}}$

$\sum_i m_i \boldsymbol{a}_i \in \{\mathrm{AI}\}$

CONTINUED No. 199 $I2_13$

Generators selected (1) $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5)

Positions

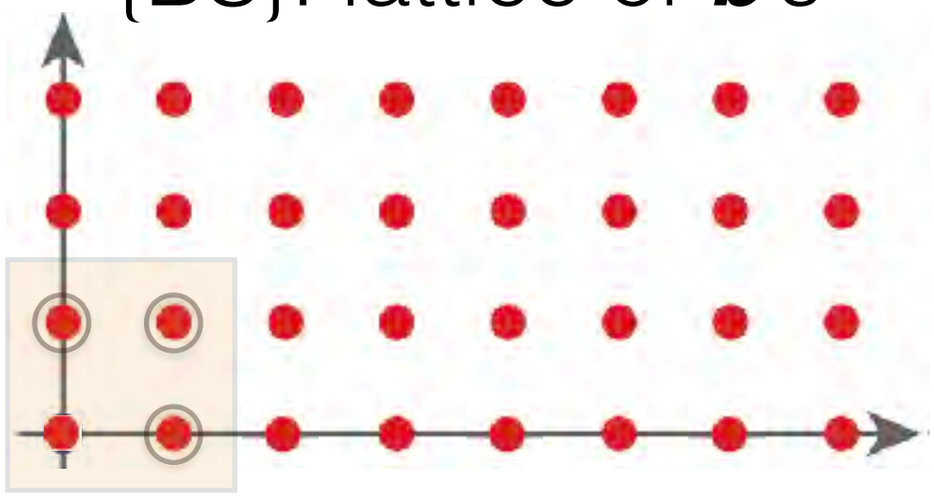
Multiplicity, Wyckoff letter, Site symmetry		Coordinates (0,0,0)+ $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$+				Reflection conditions
						h,k,l cyclically permutable
						General:
24	c 1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y},z+\frac{1}{2}$	(3) $\bar{x},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$	hkl : $h+k-l=2n$
		(5) z,x,y	(6) $z+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{y}$	(7) $\bar{z}+\frac{1}{2},\bar{x},y+\frac{1}{2}$	(8) $\bar{z},x+\frac{1}{2},\bar{y}+\frac{1}{2}$	$0kl$: $k+l=2n$
		(9) y,z,x	(10) $\bar{y},z+\frac{1}{2},\bar{x}+\frac{1}{2}$	(11) $y+\frac{1}{2},\bar{z}+\frac{1}{2},\bar{x}$	(12) $\bar{y}+\frac{1}{2},\bar{z},x+\frac{1}{2}$	hhl : $l=2n$
						$h00$: $h=2n$
						Special: no extra conditions
12	b 2 . .	$x,0,\frac{1}{4}$	$\bar{x}+\frac{1}{2},0,\frac{3}{4}$	$\frac{1}{4},z,0$	$\frac{3}{4},\bar{z}+\frac{1}{2},0$	$0,\frac{1}{4},x$ $0,\frac{3}{4},\bar{x}+\frac{1}{2}$
8	a .3.	x,x,x	$\bar{x}+\frac{1}{2},\bar{x},x+\frac{1}{2}$	$\bar{x},x+\frac{1}{2},\bar{x}+\frac{1}{2}$	$x+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{x}$	

Indicator of nontrivial band topology

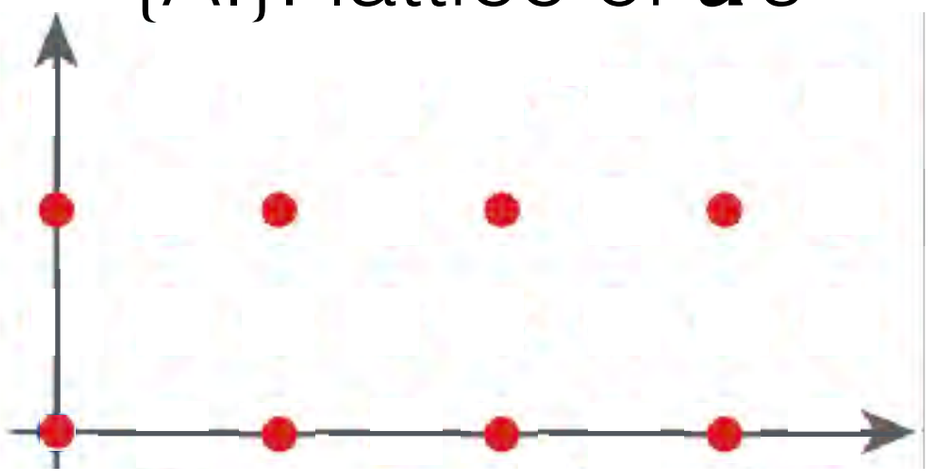
- Set of valid ***b***'s : $\{BS\} = Z^{d_{BS}}$
- Set of all ***a***'s (***b***'s corresponding to AI): $\{AI\} = Z^{d_{AI}}$

Quotient space: $X = \{BS\}/\{AI\}$ $\{BS\} > \{AI\}$

{BS}: lattice of ***b***'s



{AI}: lattice of ***a***'s



$X = Z_2 \times Z_2$

Indicator of nontrivial band topology

$$X = \{BS\}/\{AI\} = \cancel{Z^{d_{BS}-d_{AI}}} \times Z_{n1} \times Z_{n2} \times \ldots \times Z_{nN}$$

We found $d_{BS} = d_{AI}$ holds for all SGs

→ We can, in fact, compute {BS} from {AI} (easy to get)
i.e., no need to list up / solve all compatibility relations (tough)

$$\boldsymbol{b} = \sum_i q_i \boldsymbol{a}_i \in \{BS\}$$

basis vectors of{AI}

Must be integer valued Can be fractional

If necessary, one can impose
the “nonnegative”constraint at the end.

230 SGs x TRS with SOC

d	SGs
1	*1, 3, 4, 5, 6, 7, 8, 9, 16, 17, 18, 19, 20* *21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33* *34, 35, 36, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46* *76, 77, 78, 80, 91, 92, 93, 94, 95, 96, 98, 101, 102* *105, 106, 109, 110, 144, 145, 151, 152, 153, 154* *169, 170, 171, 172, 178, 179, 180, 181*
2	*79, 90, 97, 100, 104, 107, 108, 146, 155, 160, 161* *195, 196, 197, 198, 199, 208, 210, 212, 213, 214*
3	*48, 50, 52, 54, 56, 57, 59, 60, 61, 62, 68, 70, 73* *75, 89, 99, 103, 112, 113, 114, 116, 117, 118, 120* *122, 133, 142, 150, 157, 159, 173, 182, 185* *186, 209, 211*
4	*63, 64, 72, 121, 126, 130, 135, 137, 138, 143, 149* *156, 158, 168, 177, 183, 184, 207, 218, 219, 220*
5	*11, 13, 14, 15, 49, 51, 53, 55, 58, 66, 67, 74, 81* *82, 86, 88, 111, 115, 119, 134, 136, 141, 167* *217, 228, 230*
6	*69, 71, 85, 125, 129, 132, 163, 165, 190, 201* *203, 205, 206, 215, 216, 222*
7	*12, 65, 84, 128, 131, 140, 188, 189, 202, 204, 223*
8	*124, 127, 148, 166, 193, 200, 224, 226, 227*
9	*2, 10, 47, 87, 139, 147, 162, 164, 176, 192, 194*
10	*174, 187*
11	*225, 229*
13	*83, 123*
14	*175, 191, 221*

X_{BS}	SGs
$\mathbb{Z}_2$	*81, 82, 111, 112, 113, 114, 115, 116, 117* *118, 119, 120, 121, 122, 215, 216, 217* *218, 219, 220*
$\mathbb{Z}_3$	*188, 190*
$\mathbb{Z}_4$	*52, 56, 58, 60, 61, 62, 70, 88, 126* *130, 133, 135, 136, 137, 138, 141, 142* *163, 165, 167, 202, 203, 205, 222, 223* *227, 228, 230*
$\mathbb{Z}_8$	*128, 225, 226*
$\mathbb{Z}_{12}$	*176, 192, 193, 194*
$\mathbb{Z}_2 \times \mathbb{Z}_4$	*14, 15, 48, 50, 53, 54, 55, 57, 59* *63, 64, 66, 68, 71, 72, 73, 74, 84, 85* *86, 125, 129, 131, 132, 134, 147, 148* *162, 164, 166, 200, 201, 204, 206, 224*
$\mathbb{Z}_2 \times \mathbb{Z}_8$	*87, 124, 139, 140, 229*
$\mathbb{Z}_3 \times \mathbb{Z}_3$	*174, 187, 189*
$\mathbb{Z}_4 \times \mathbb{Z}_8$	*127, 221*
$\mathbb{Z}_6 \times \mathbb{Z}_{12}$	*175, 191*
$(Z_2)^2 \times \mathbb{Z}_4$	*11, 12, 13, 49, 51, 65, 67, 69*
$\mathbb{Z}_2 \times \mathbb{Z}_4 \times \mathbb{Z}_8$	*83, 123*
$(\mathbb{Z}_2)^3 \times \mathbb{Z}_4$	*2, 10, 47*

230 SGs x TRS without SOC

d	SGs
1	*1, 4, 7, 9, 19, 29, 33, 76, 78, 144, 145, 169, 170*
2	*8, 31, 36, 41, 43, 80, 92, 96, 110, 146, 151, 198*
3	*5, 6, 18, 20, 26, 30, 32, 34, 40, 45, 46, 61, 106 109, 151, 152, 153, 154, 159, 160, 171, 172, 173, 178, 179, 199, 212, 213*
4	*24, 28, 37, 39, 60, 62, 77, 79, 91, 95, 102, 104 143, 155, 157, 158, 185, 186, 196, 197, 210*
5	*3, 14, 17, 27, 42, 44, 52, 56, 57, 94, 98, 100, 101 108, 114, 122, 150, 156, 182, 214, 220*
6	*11, 15, 35, 38, 54, 70, 73, 75, 88, 90, 103, 105, 107 113, 142, 149, 167, 168, 184, 195, 205, 219*
7	*13, 22, 23, 59, 64, 68, 82, 86, 117, 118, 120, 130, 163 165, 180, 181, 203, 206, 208, 209, 211, 218, 228, 230*
8	*21, 58, 63, 81, 85, 97, 116, 133, 135, 137, 148, 183, 190, 201, 217*
9	*2, 25, 48, 50, 53, 55, 72, 99, 121, 126, 138, 141 147, 188, 207, 216, 222*
10	*12, 74, 93, 112, 119, 176, 177, 202, 204, 215*
11	*66, 84, 128, 136, 166, 227*
12	*51, 87, 89, 115, 129, 134, 162, 164, 174, 189, 193, 223, 226*
13	*16, 67, 111, 125, 194, 224*
14	*49, 140, 192, 200*
15	*10, 69, 71, 124, 127, 132, 187*
17	*225, 229*
18	*65, 83, 131, 139, 175*
22	*221*
24	*191*
27	*47, 123*

X_{BS}	SGs
$\mathbb{Z}_2$	*3, 11, 14, 27, 37, 48, 49, 50, 52, 53, 54, 56 58, 60, 66, 68, 70, 75, 77, 82, 85, 86, 88 103, 124, 128, 130, 162, 163, 164, 165, 166 167, 168, 171, 172, 176, 184, 192, 201, 203*
$(\mathbb{Z}_2)^2$	*12, 13, 15, 81, 84, 87*
$\mathbb{Z}_2 \times \mathbb{Z}_4$	*147, 148*
$(\mathbb{Z}_2)^3$	*10, 83, 175*
$(\mathbb{Z}_2)^3 \times \mathbb{Z}_4$	*2*

2D layer groups

Supplementary Table 17. Symmetry-based indicators of band topology for quasi-two-dimensional systems with significant spin-orbit coupling and time-reversal symmetry.

X_{BS}	Layer groups
$\mathbb{Z}_2$	2, 6, 7, 14, 15, 16, 17, 18, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 47, 48, 52, 62, 64, 66, 71, 72
$\mathbb{Z}_3$	74, 78, 79
$\mathbb{Z}_4$	51, 61, 63
$\mathbb{Z}_6$	75, 80

X_{BS}: the quotient group between the group of band structures and atomic insulators.

Supplementary Table 18. Symmetry-based indicators of band topology for quasi-two-dimensional systems with negligible spin-orbit coupling and time-reversal symmetry.

X_{BS}	Layer groups
$\mathbb{Z}_2$	2, 3, 7, 49, 50, 52, 66, 73
$\mathbb{Z}_2 \times \mathbb{Z}_2$	6, 51, 75

X_{BS}: the quotient group between the group of band structures and atomic insulators.

Example 1:
Representation-enforced
Quantum Band Insulator

Inversion &TR symmetric 3D system (SG2 & TRS)

$$X = Z_2 \times Z_2 \times Z_2 \times Z_4$$

weak TI strong TI + α

Two copies of TI
No surface Dirac / no magnetoelectric response.

Still topologically nontrivial (residual entanglement)
The experimental signatures are future work.

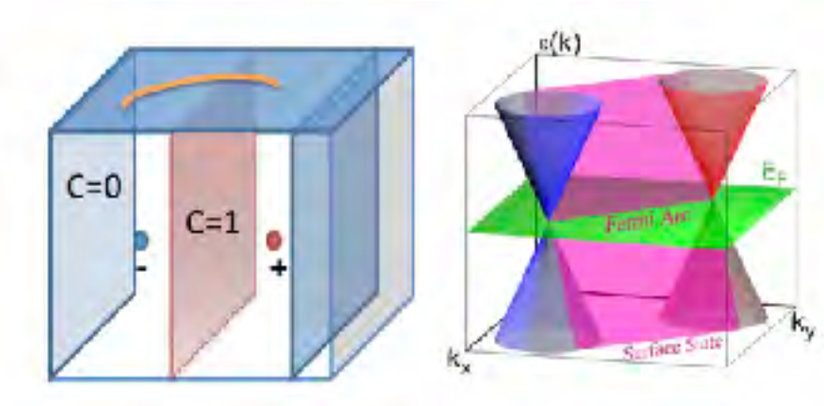
Example 2:
Representation-enforced Semi Metal

Inversion symmetric but TR broken 3D system (SG2)

$$X = Z_2 \times Z_2 \times Z_2 \times Z_4$$

Weyl SM

A. Turner, …, A. Vishwanath (2010)



{BS}: “band structure” can be *band insulator*
or *semimetal (band touching at generic points in BZ)*

(We demanded band gap only at high-symmetric momenta)

Example 3: *Filling-enforced* Quantum Band Insulator

H. C. Po, HW, M.P. Zaletel & A. Vishwanath, Science Adv. 2(4), e1501782 (2016)

- Filling mismatch between {BS} and {AI}.

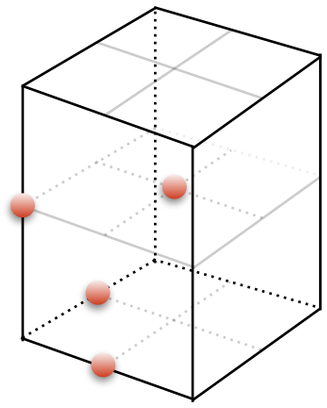
a = (2,0,4,0,2,0,0,2,6), filling ν

→ ***a***/2 = (1,0,2,0,1,0,0,1,3), filling ν/2

- e.g., SG106 (spinless, no TR). AI has filling 4n.

→ BI at filling 4n+2 must be nontrivial.

- No (symmetric&localized) Wannier orbitals



Summary

- Combination of irreps at high-sym momenta *indicates* nontrivial band topology (re/fe/le-QBI/SM)

- $\boldsymbol{b} = (n_{\boldsymbol{k}1}{}^1, n_{\boldsymbol{k}1}{}^2, \ldots n_{\boldsymbol{k}2}{}^1, n_{\boldsymbol{k}2}{}^2, \ldots)$

Set of valid $\boldsymbol{b}$'s: $\{BS\} = Z^{dBS}$

Set of $\boldsymbol{b}$'s corresponding to AI: $\{AI\} = Z^{dAI}$

- $X = \{BS\}/\{AI\} = Z_{n1} \times Z_{n2} \times \ldots \times Z_{nN}$

- Experimental signatures for each X?

X_{BS}	SGs
$\mathbb{Z}_2$	*81, 82, 111, 112, 113, 114, 115, 116, 117 118, 119, 120, 121, 122, 215, 216, 217 218, 219, 220*
$\mathbb{Z}_3$	*188, 190*
$\mathbb{Z}_4$	*52, 56, 58, 60, 61, 62, 70, 88, 126 130, 133, 135, 136, 137, 138, 141, 142 163, 165, 167, 202, 203, 205, 222, 223 227, 228, 230*
$\mathbb{Z}_8$	*128, 225, 226*
$\mathbb{Z}_{12}$	*176, 192, 193, 194*
$\mathbb{Z}_2 \times \mathbb{Z}_4$	*14, 15, 48, 50, 53, 54, 55, 57, 59 63, 64, 66, 68, 71, 72, 73, 74, 84, 85 86, 125, 129, 131, 132, 134, 147, 148 162, 164, 166, 200, 201, 204, 206, 224*
$\mathbb{Z}_2 \times \mathbb{Z}_8$	*87, 124, 139, 140, 229*
$\mathbb{Z}_3 \times \mathbb{Z}_3$	*174, 187, 189*
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$\mathbb{Z}_6 \times \mathbb{Z}_{12}$	*175, 191*
$(\mathbb{Z}_2)^2 \times \mathbb{Z}_4$	*11, 12, 13, 49, 51, 65, 67, 69*
$\mathbb{Z}_2 \times \mathbb{Z}_4 \times \mathbb{Z}_8$	*83, 123*
$(\mathbb{Z}_2)^3 \times \mathbb{Z}_4$	*2, 10, 47*