

Interplay of **symmetry** & **topology** in noninteracting (and interacting) systems

Haruki Watanabe
University of Tokyo

Interplay of **symmetry** & **topology**

- Symmetry protects topology e.g. Quantum Spin Hall

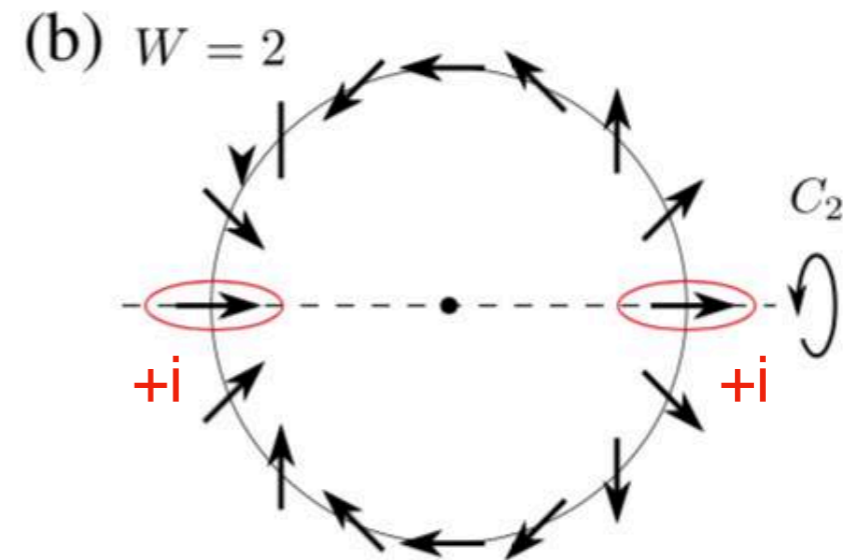
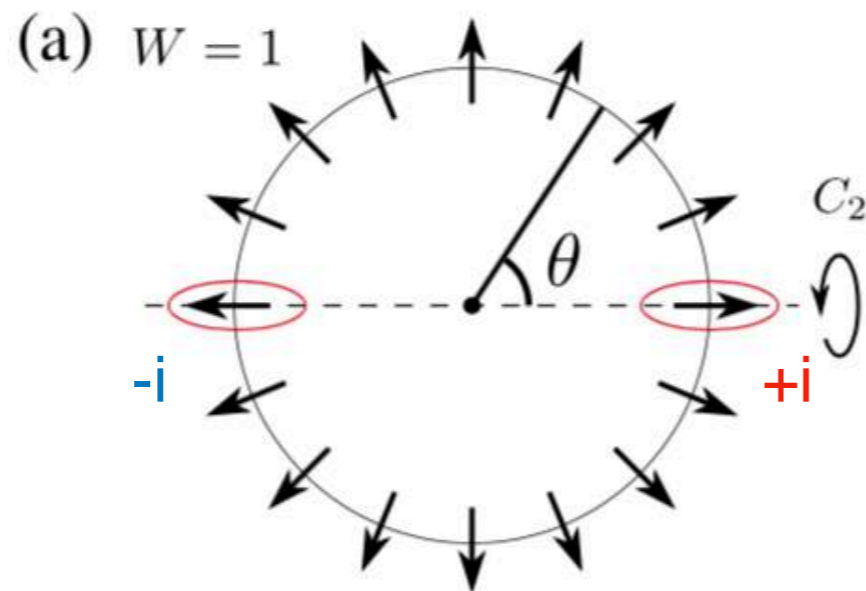
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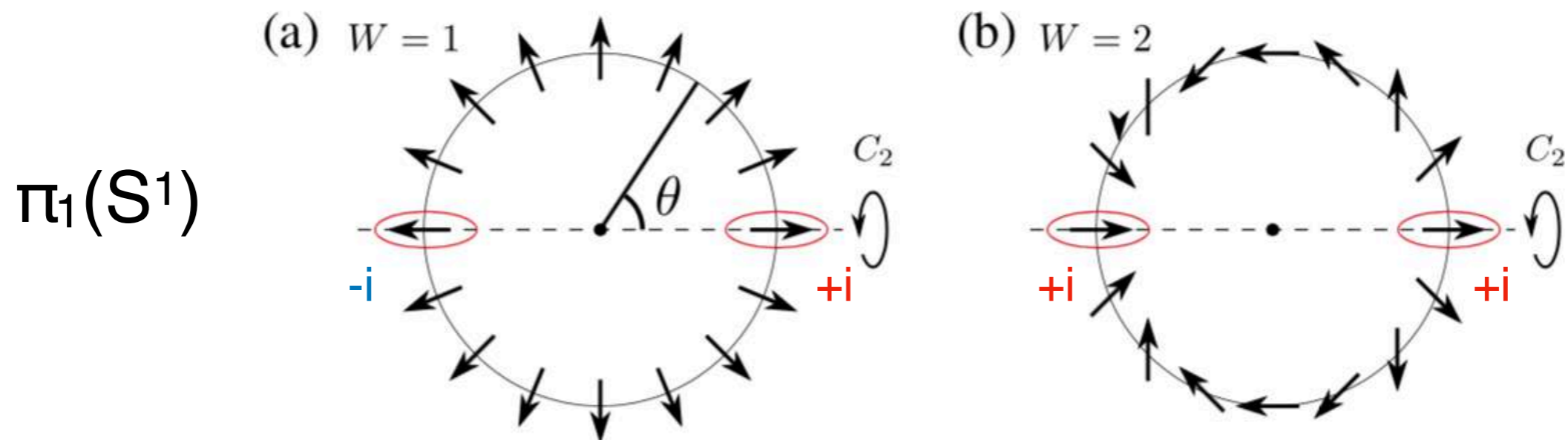
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$\pi_1(S^1)$



Interplay of symmetry & topology

- Symmetry protects topology e.g. Quantum Spin Hall
- Symmetry detects topology



$W \bmod 2$ can be seen from the product of two rotation eigenvalues!

Fu-Kane formula

- Z_2 index for Quantum Spin Hall insulators (2D, TR)

Requires a careful gauge fixing and integration of Pfaffian in k space

Fu-Kane formula

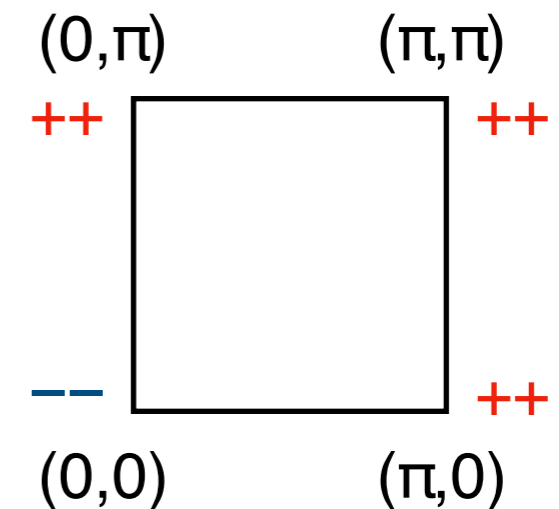
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- With additional **inversion symmetry**

Fu-Kane formula: $\nu = \prod_{k=\text{TRIMs}} \xi_k = \pm 1$

Easy & helpful for material search!



Combination of **inversion eigenvalues** indicates **Z_2 QSH**

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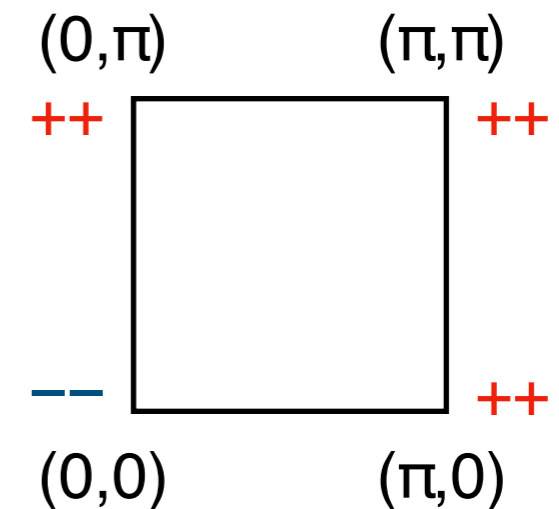
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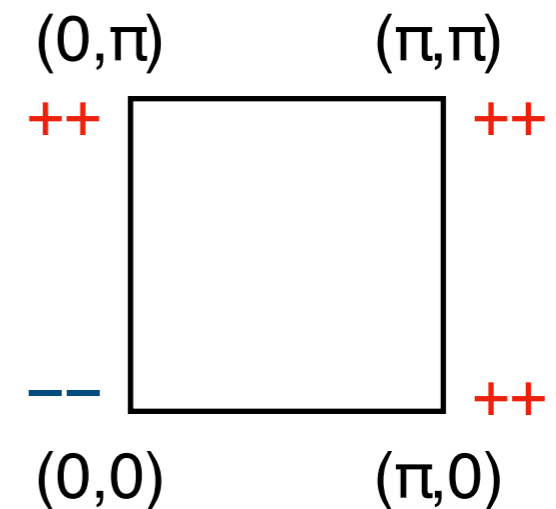
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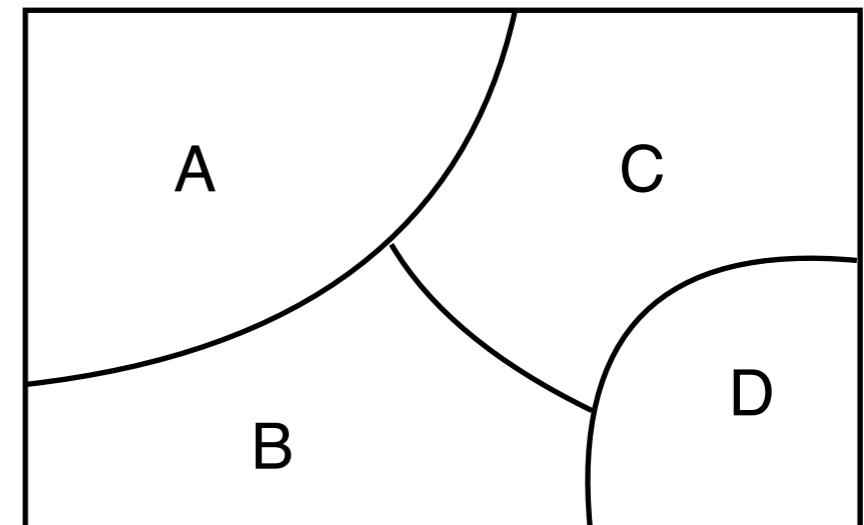
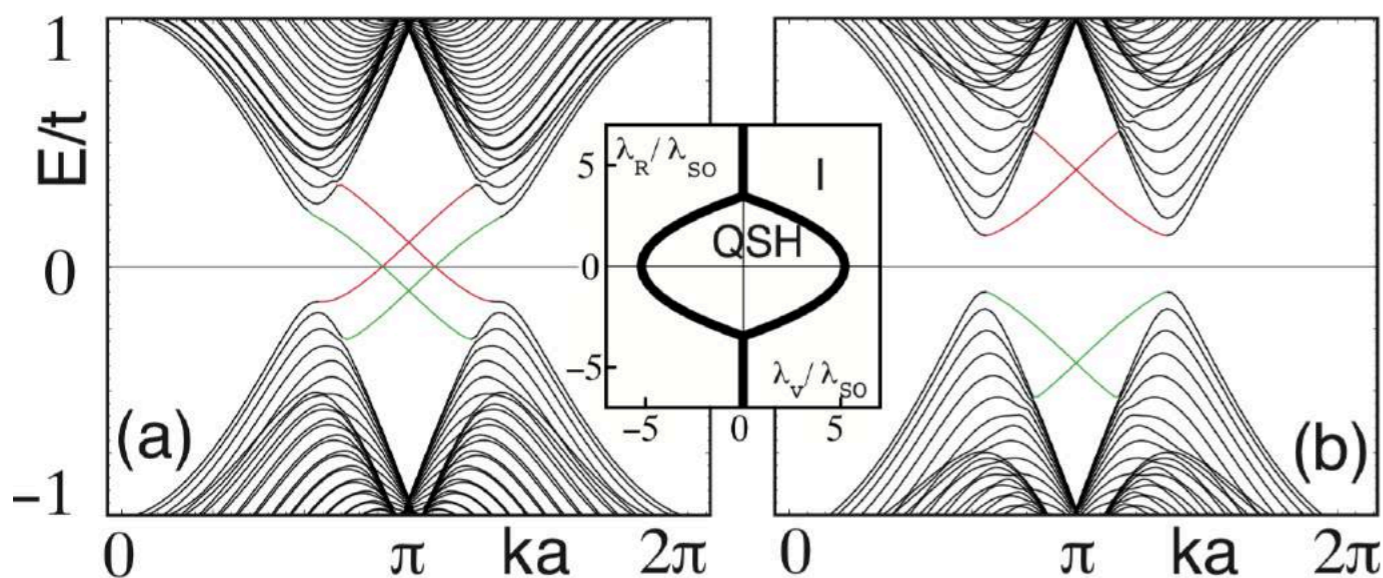


Irreducible representations of a more general space group
Combination of ~~inversion eigenvalues~~ indicates ~~Z_2 QSH~~

more general topology including HOTI

“topological” insulators

1. Presence of protected gapless edge/surface states
 2. Winding number (e.g. Chern number, Z2 QSH index)
 3. Obstruction in adiabatically connecting to trivial states
- Most general definition / applicable to interacting systems



Plan of my talk

- Basics of symmetry indicators
- What can we “see” from it?
 1. Conventional topological insulators (Chern, Z_2 TI, etc)
 2. Higher-order topological insulators
 3. Weyl semimetals
 4. Fragile topology
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Characterizing band structure by irreducible representations

Po-Vishwanath-Watanabe, Nat. Commun. (2017)

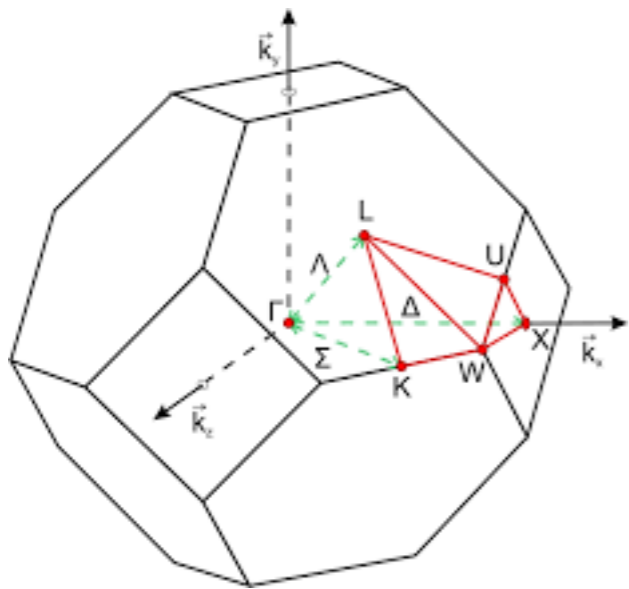
Related works:

Bradlyn-...-Bernevig (2017)

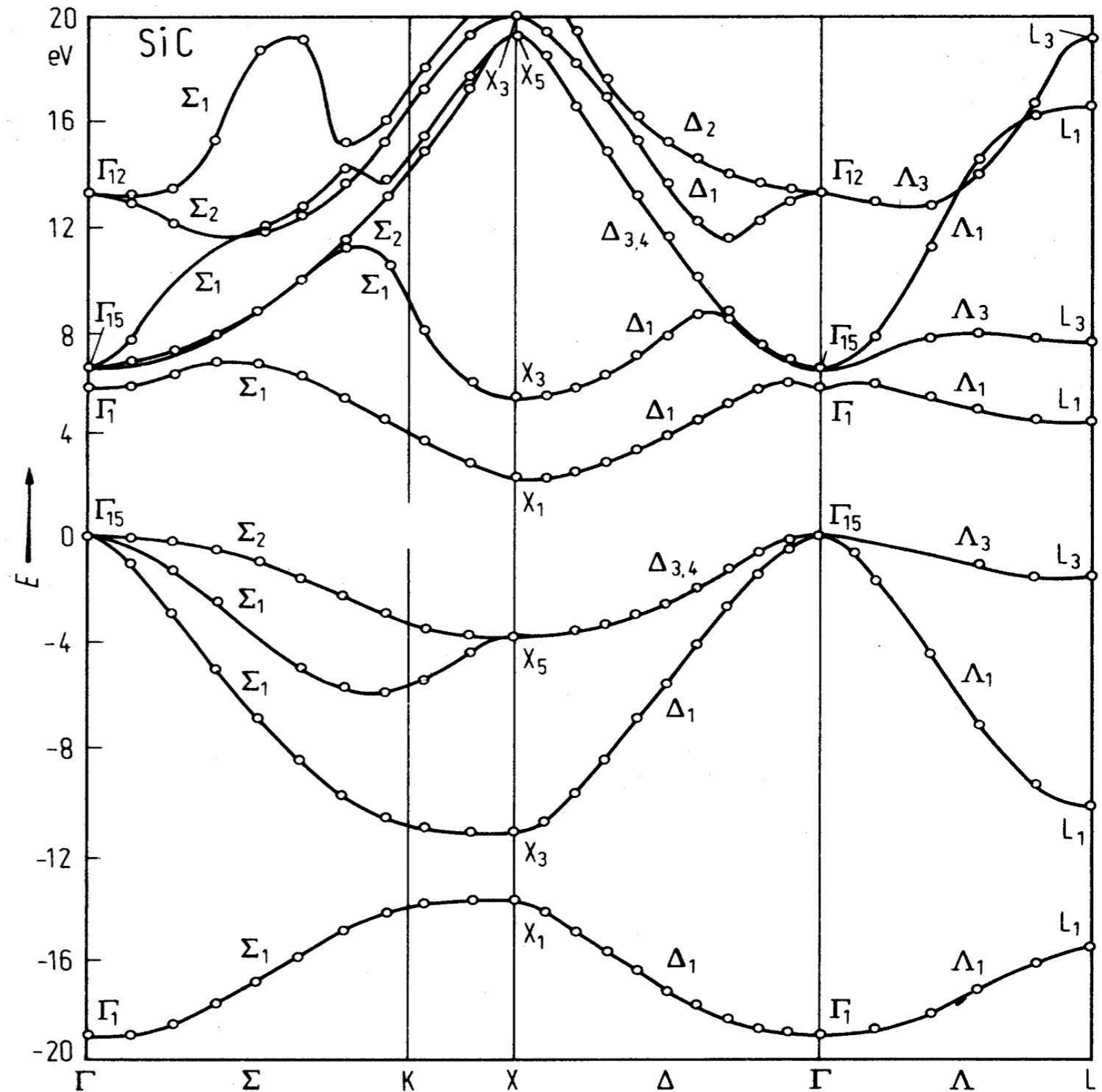
Shiozaki-Sato-Gomi (2018)

Song-...-Fang (2018)

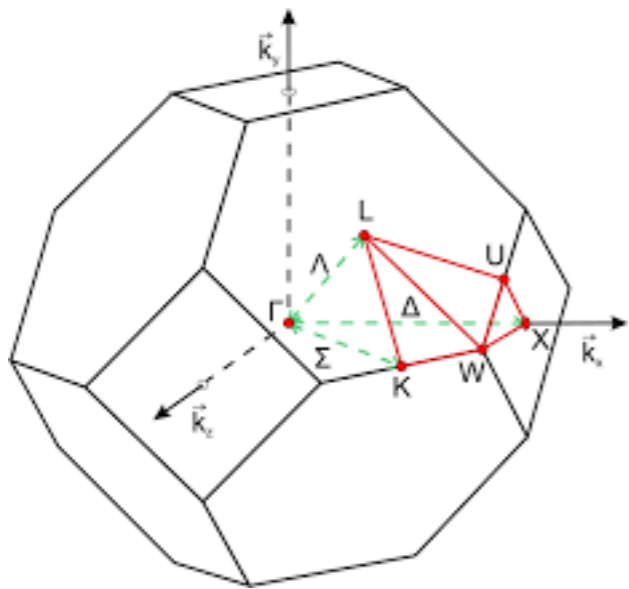
Representations in band structures



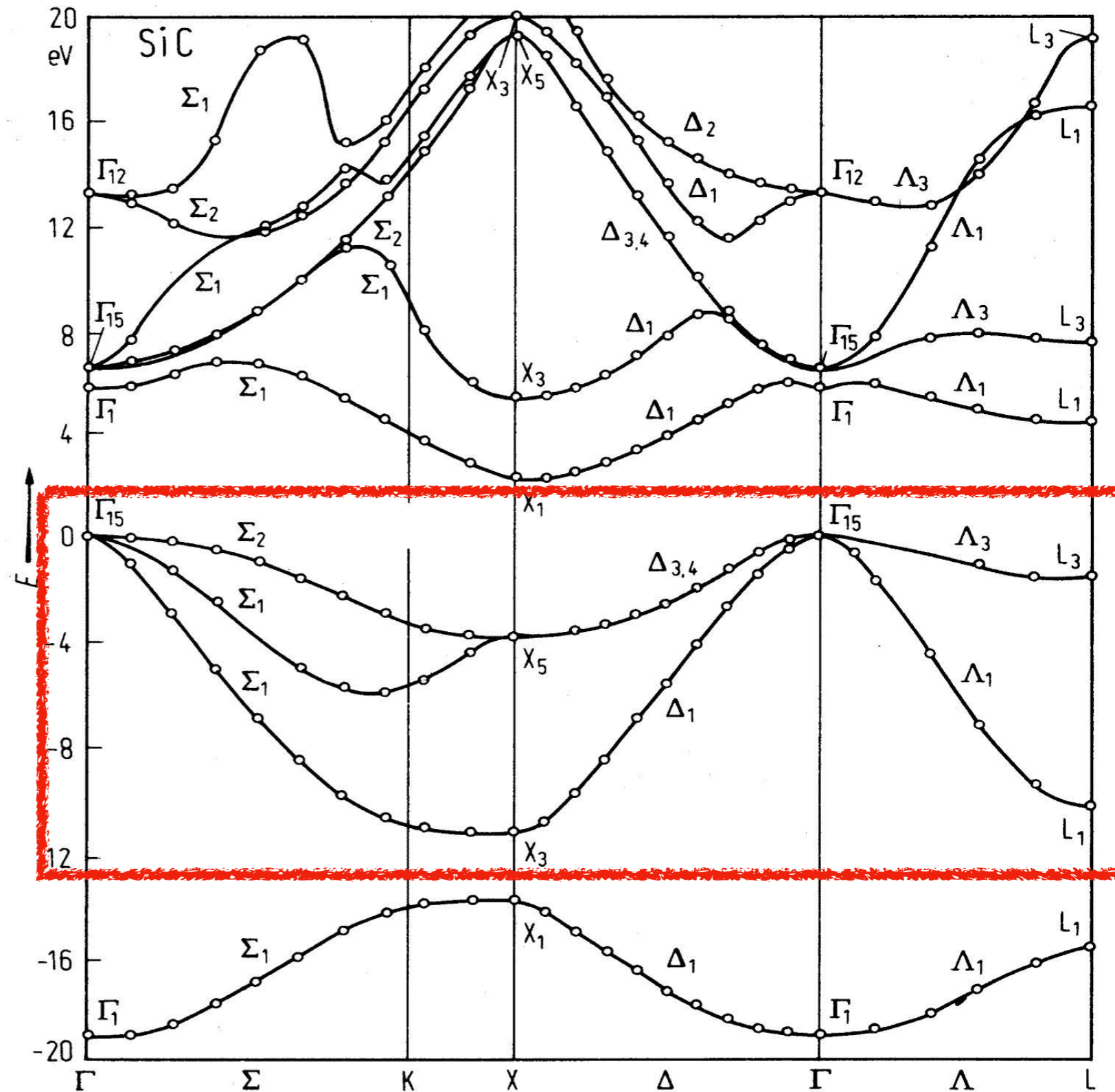
Hemstreet & Fong (1974)



Representations in band structures



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Step-by-step process

Given symmetry setting (e.g., space group G , TR, spin-orbit)

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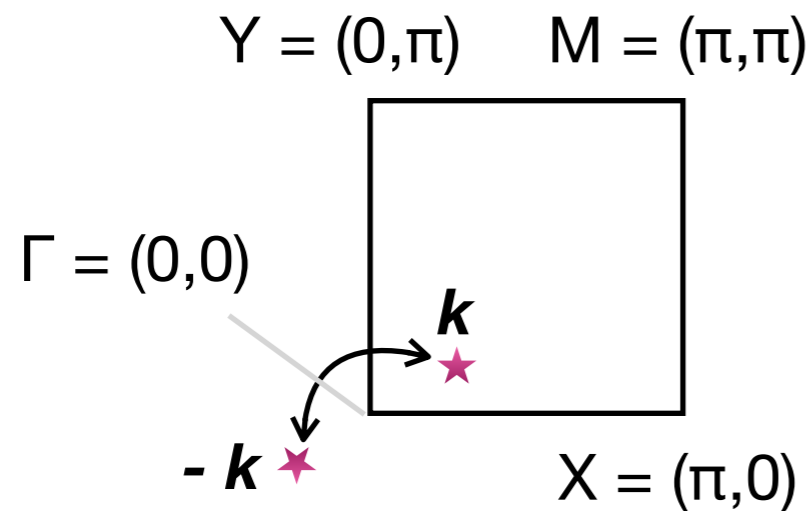
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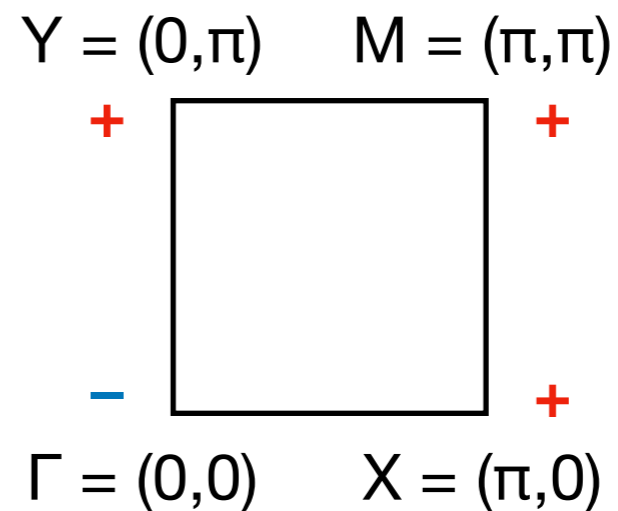
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5. Form a vector $\mathbf{b} = (n_{k_1^1}, n_{k_1^2}, \dots, n_{k_2^1}, n_{k_2^2}, \dots)$

Example: 2D lattice with inversion symmetry



Inversion $\mathcal{I}^2 = +1$
 → eigenvalues **+1** or **-1**



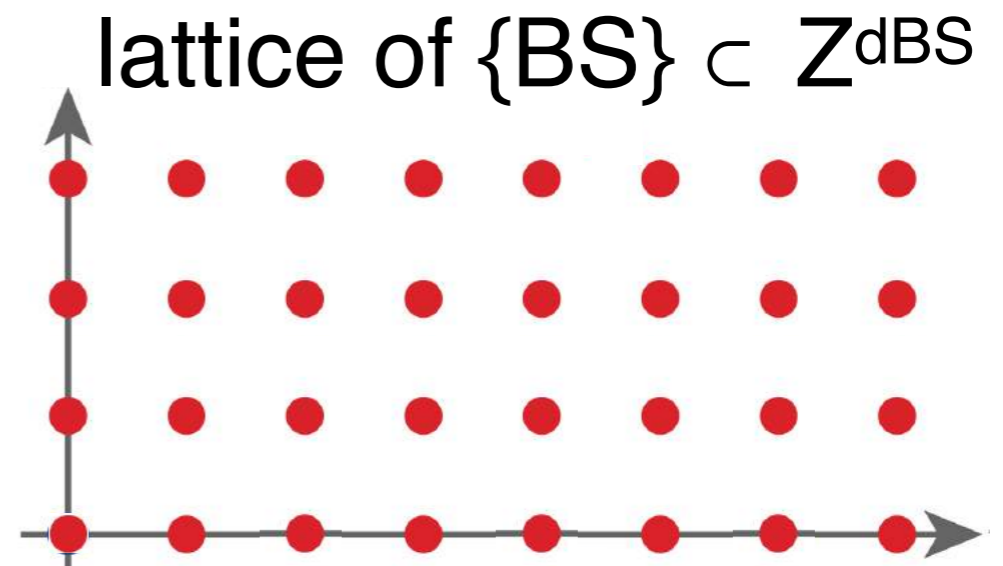
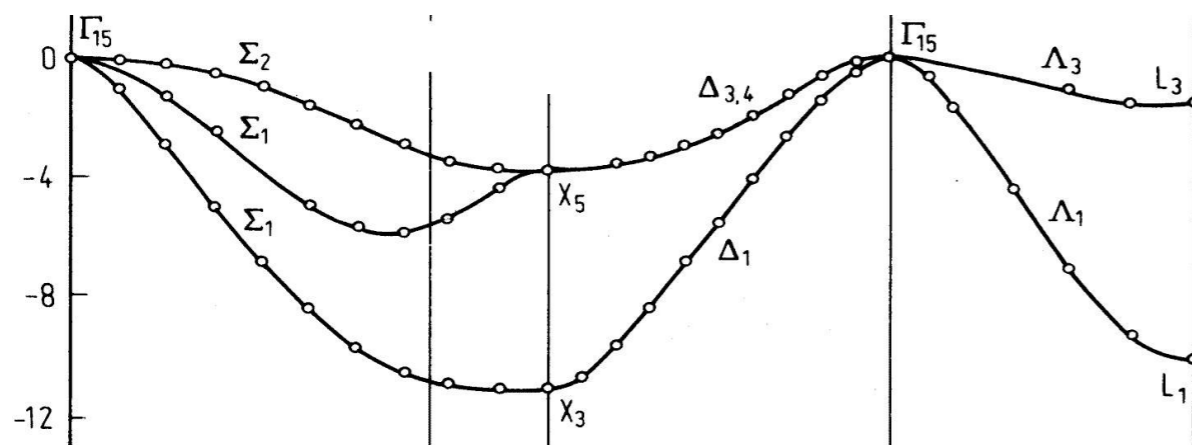
$(\Gamma, X, Y, M) : (-, +, +, +)$

$\mathbf{b} = (0, 1, 1, 0, 1, 0, 1, 0)$

Band structure space {BS}

- Consider a vector $\mathbf{b} = \{n_k^a\} = (n_{k_1^1}, n_{k_1^2}, \dots, n_{k_2^1}, n_{k_2^2}, \dots)$ satisfying all compatibility relations at high-sym momenta
- Form a set \mathbf{b} 's (band structure space) :

$$\{\text{BS}\} = \{ \mathbf{b} = \{n_k^a\} \mid \text{satisfying compatibility relations} \} \subset \mathbb{Z}^{\text{dBS}}$$

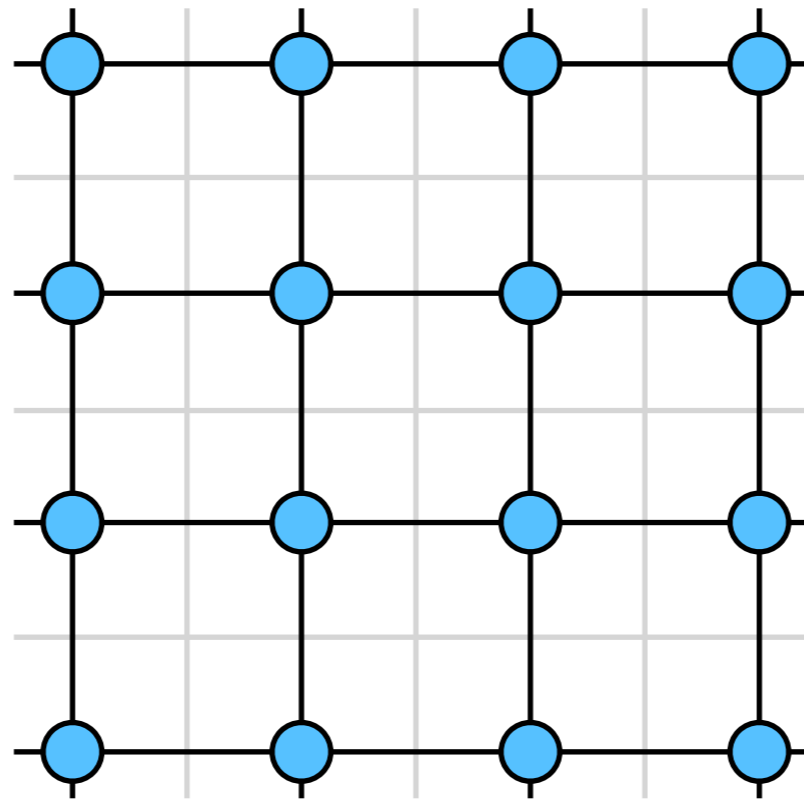


Trivial subset of $\{BS\}$

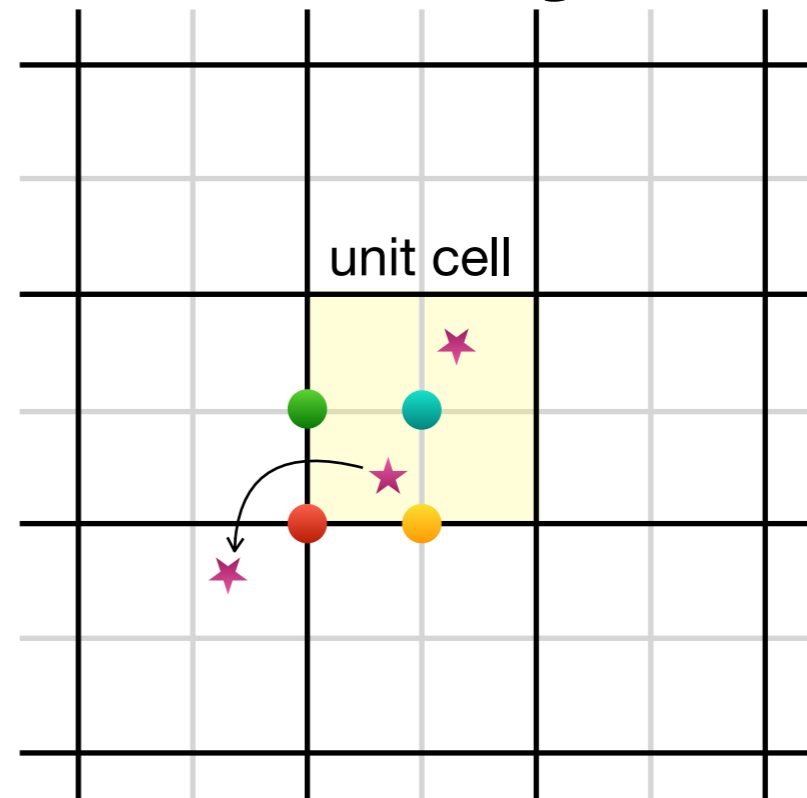
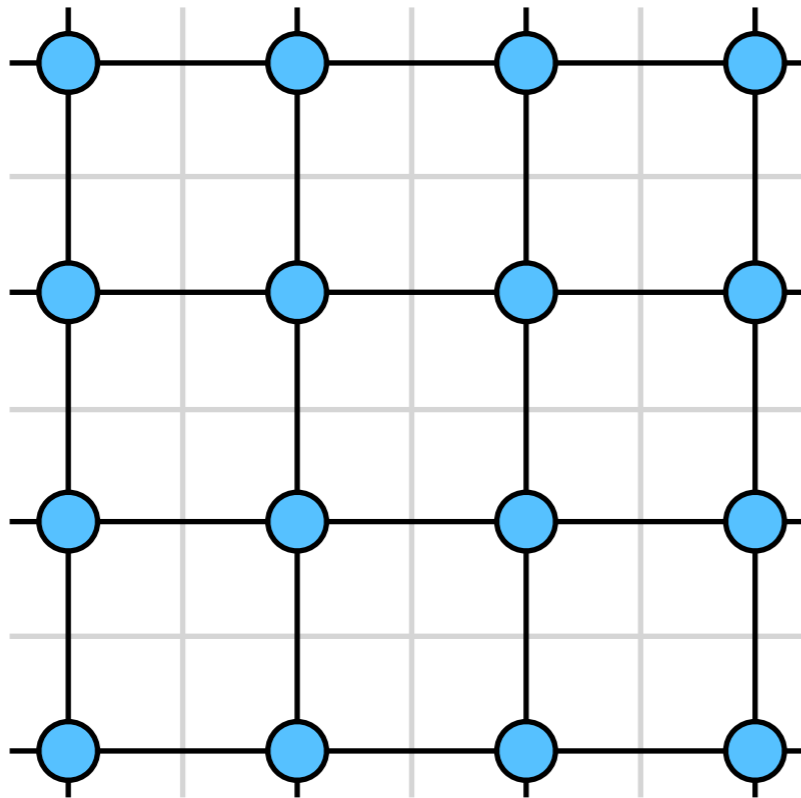
Atomic Insulators

TB model but no hopping (trivial flat bands)

Product state in real space (trivial) \Leftrightarrow Wannier orbitals



Example: 2D lattice with inversion symmetry



We have to specify the position \mathbf{x} and the orbital type

1. Choose \mathbf{x} in unit cell.

e.g. $\mathbf{x} = \bullet$

2. Find little group (site-symmetry) $G_{\mathbf{x}}$.

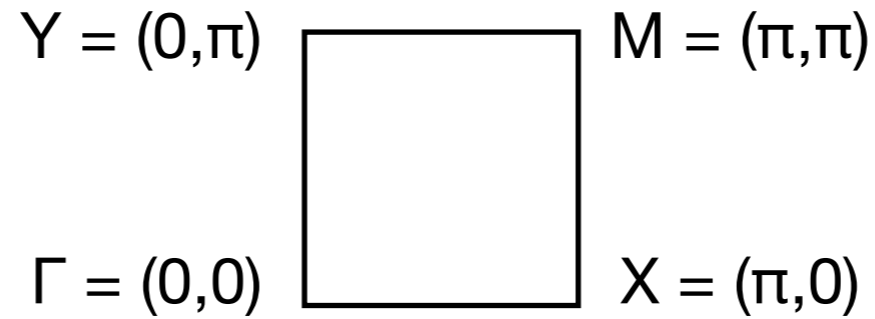
$G_{\mathbf{x}} = \{e, I\}$ at $\mathbf{x} = \bullet$

3. Choose an orbit (an irrep of $G_{\mathbf{x}}$).

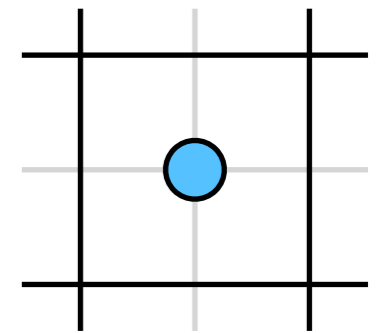
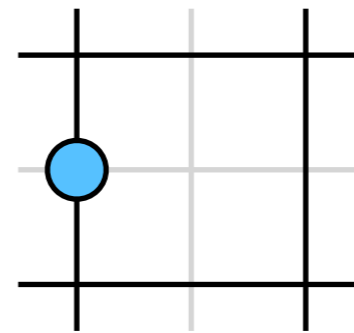
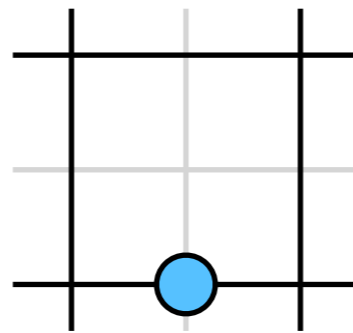
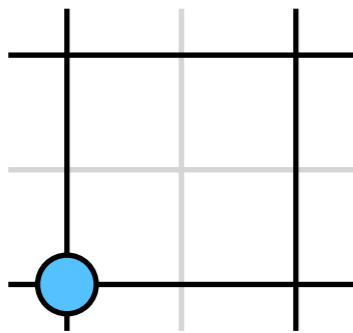
\bullet ($l = +1$) $\bullet\bullet$ ($l = -1$)

Irrep contents of AI

Momentum space



Real space

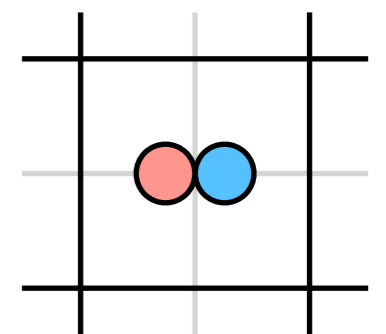
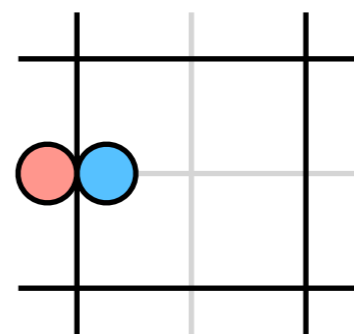
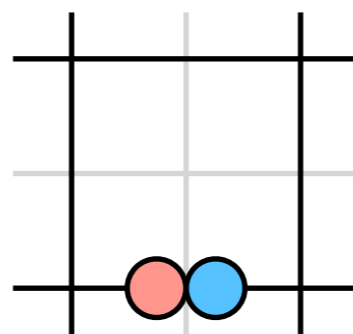
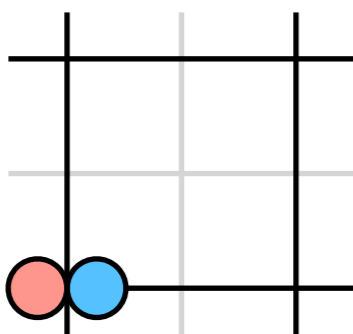


$(\Gamma, X, Y, M) :$ $(+, +, +, +)$

$(+, -, +, -)$

$(+, +, -, -)$

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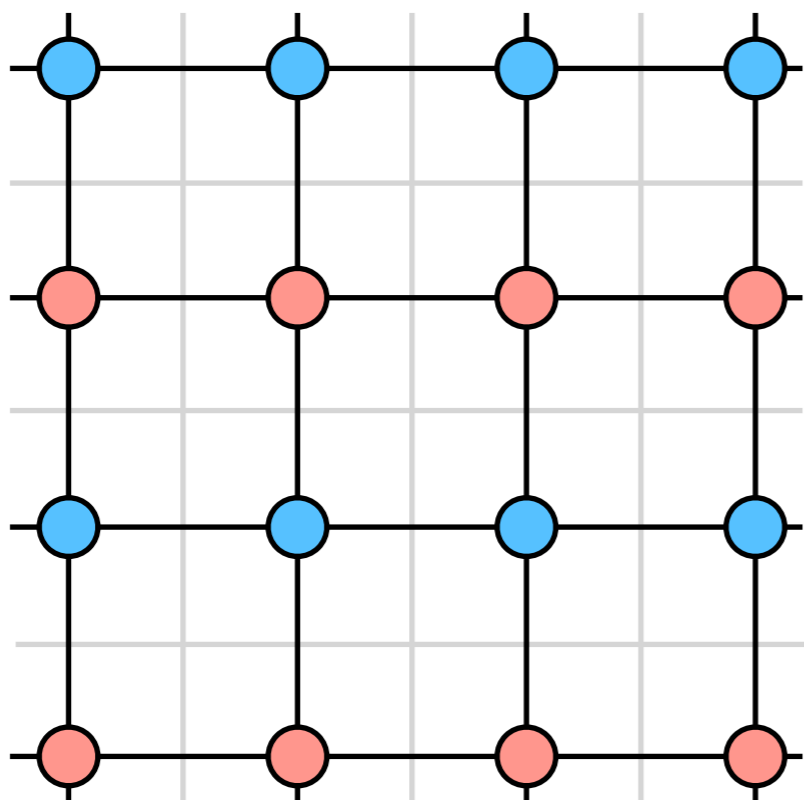
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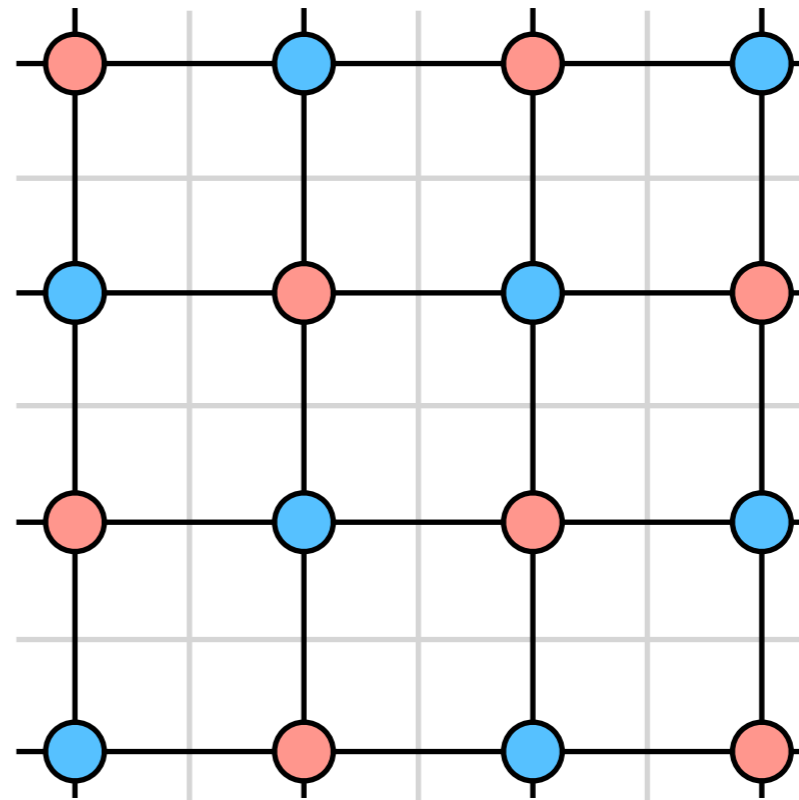
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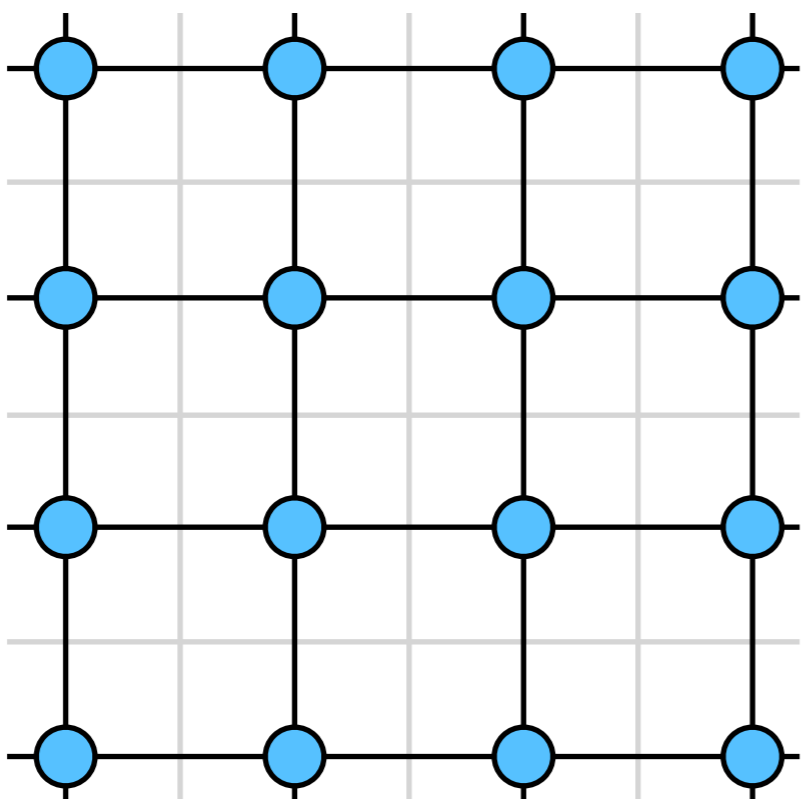
$k = (0, \pi)$
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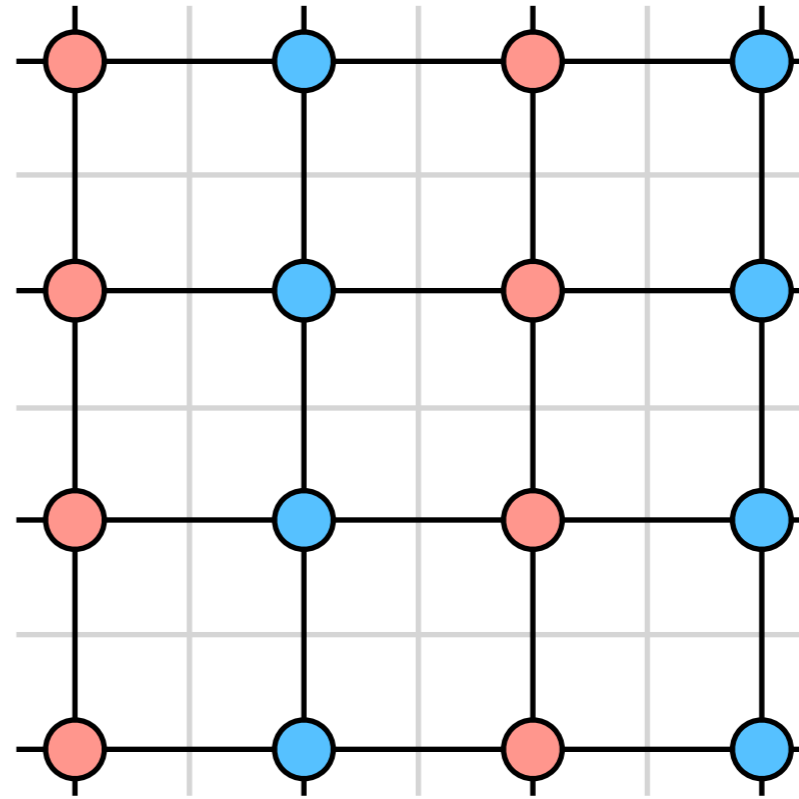
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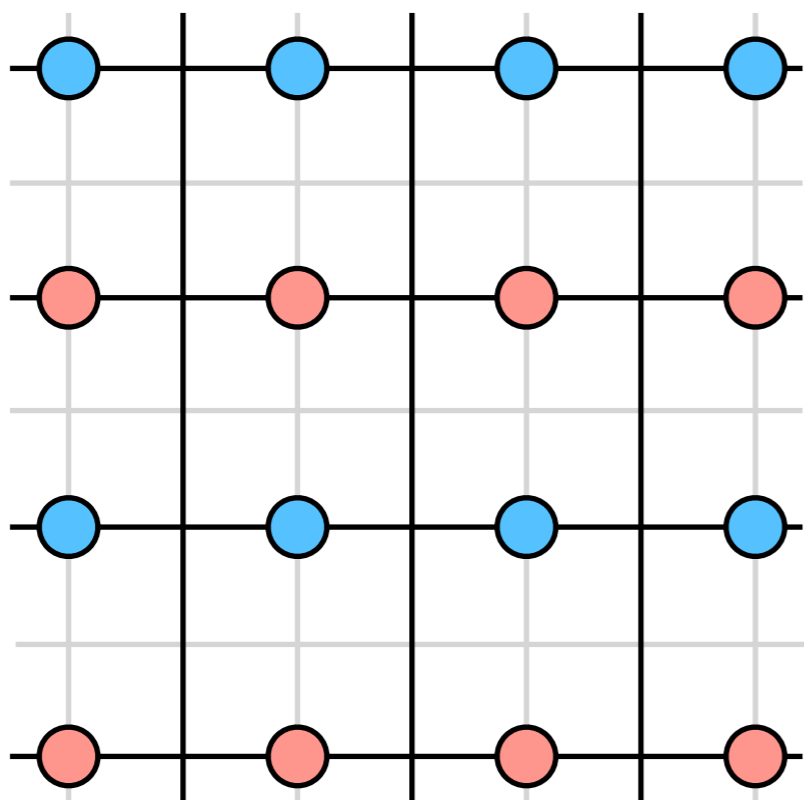
$k = (0, 0)$
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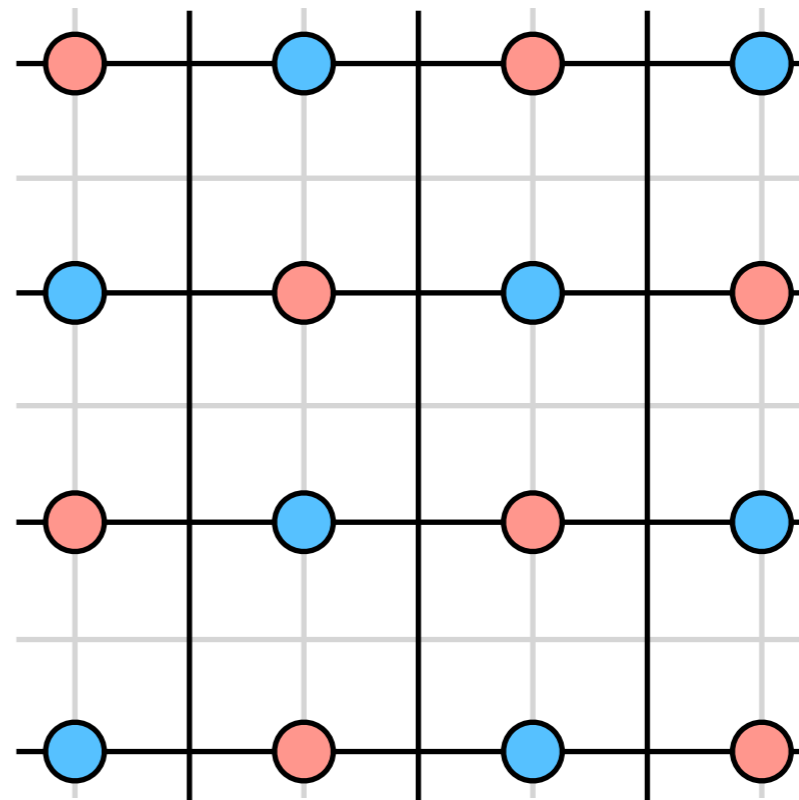
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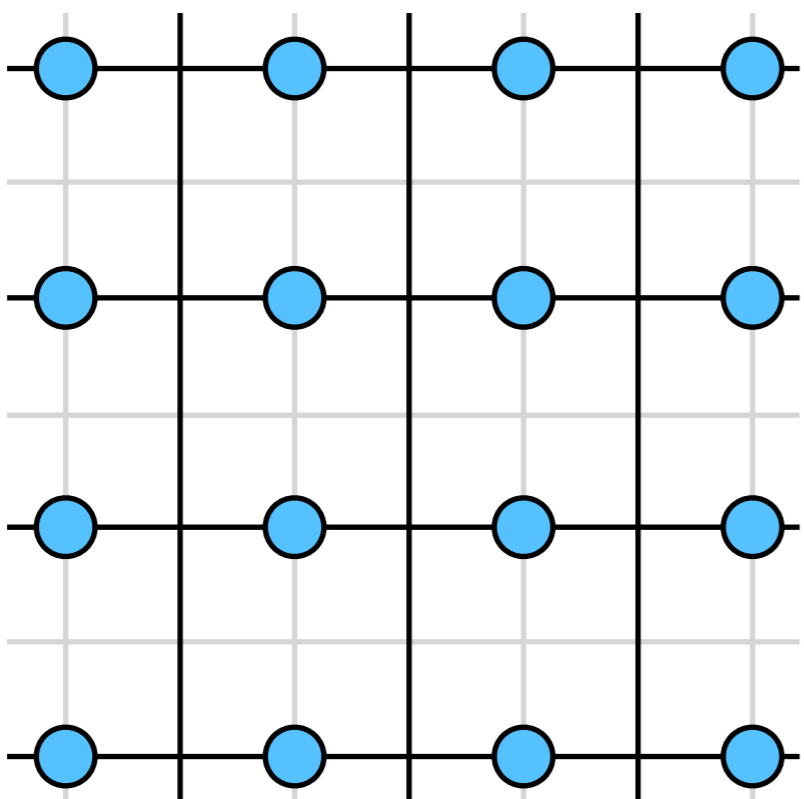
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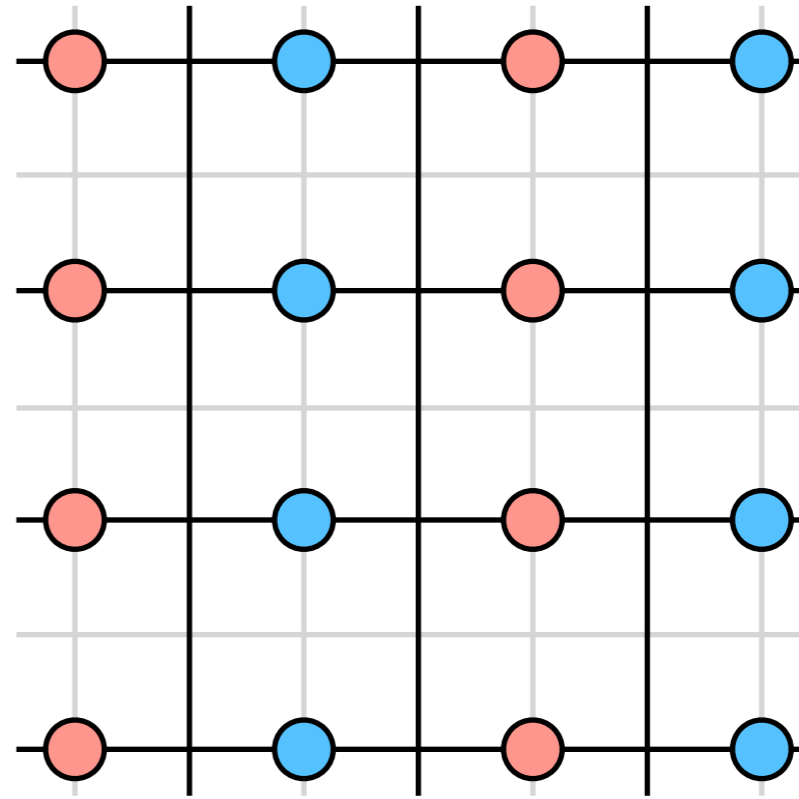
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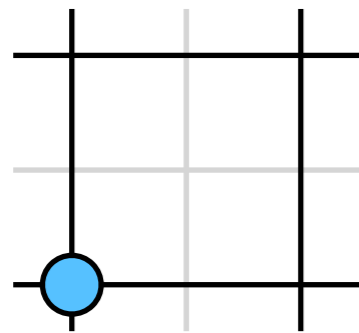
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Atomic insulator space $\{AI\}$

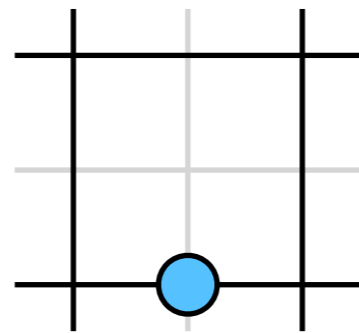
- Consider a vector $\mathbf{a} = \{n_k^a\} = (n_{k_1^1}, n_{k_1^2}, \dots, n_{k_2^1}, n_{k_2^2}, \dots)$ corresponding to atomic insulators. They automatically satisfy all compatibility relations.
- Form the set \mathbf{a} 's (atomic insulator space) :

$$\{AI\} = \{ \mathbf{a} = \{n_k^a\} \mid \text{corresponding to AI} \} \subset \mathbb{Z}^{d_{AI}}$$



$(+, +, +, +)$

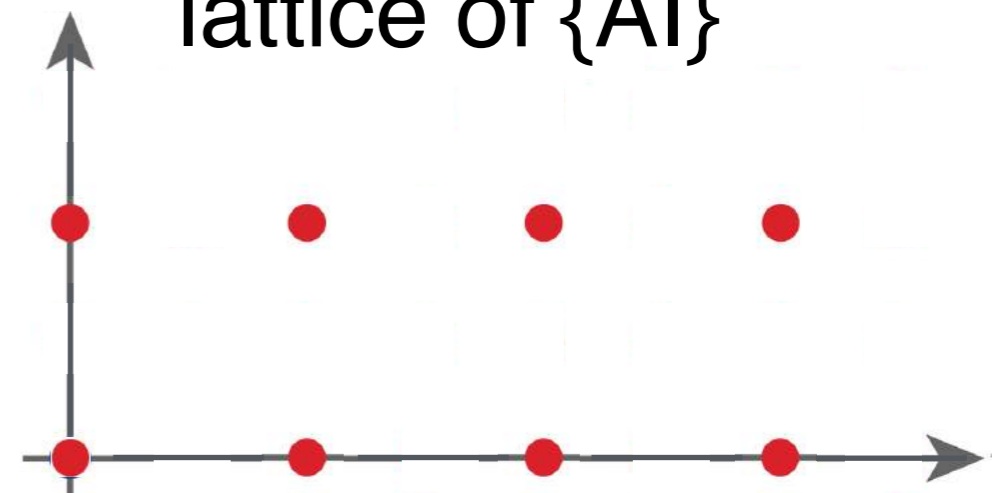
$$\mathbf{a}_1 = (1, 0, 1, 0, 1, 0, 1, 0)$$



$(+, -, +, -)$

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

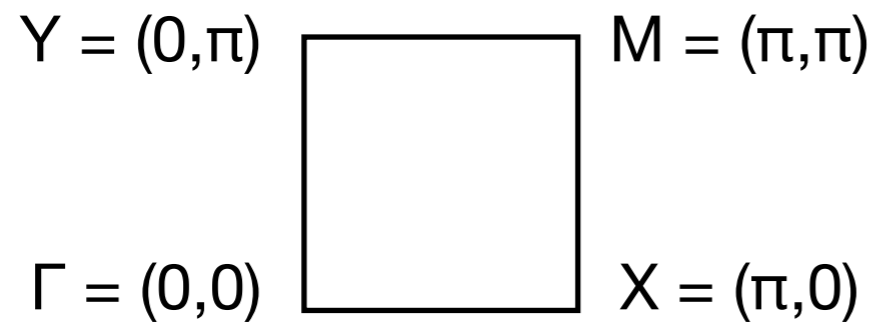
lattice of $\{AI\}$



Diagnosing the topology

Band Structures **{BS}**: set of ***b***'s

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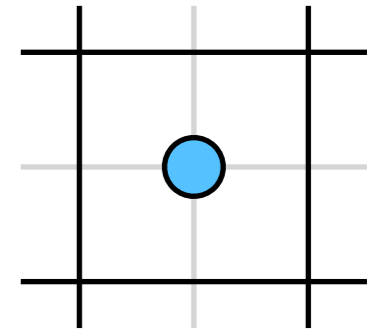
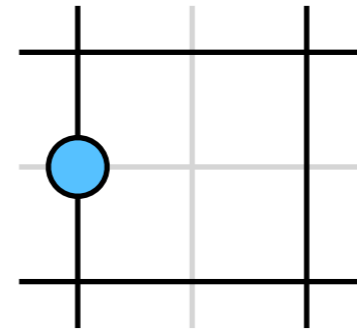
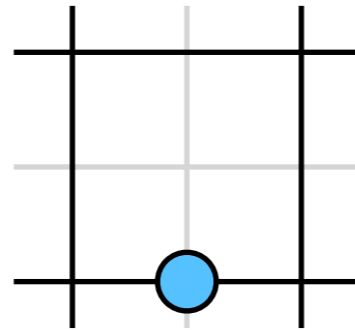
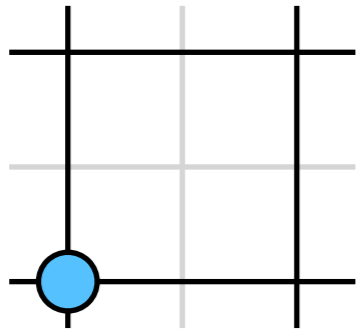


$$\mathbf{b}_2 = (++, +-, +-, ++)$$

$$\mathbf{b}_3 = (+, +, +, -)$$

$$\mathbf{b}_4 = (++, ++, ++, --)$$

Atomic Insulators **{AI}**: set of ***a***'s

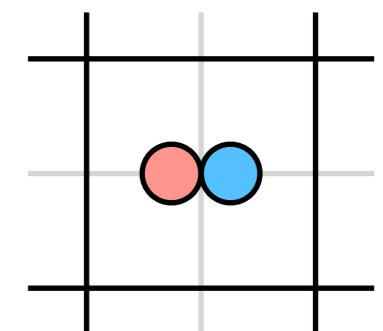
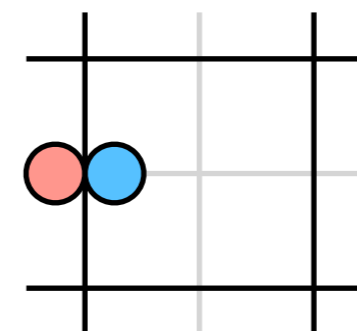
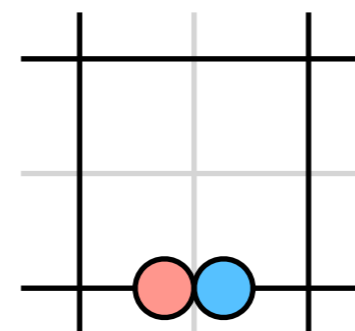
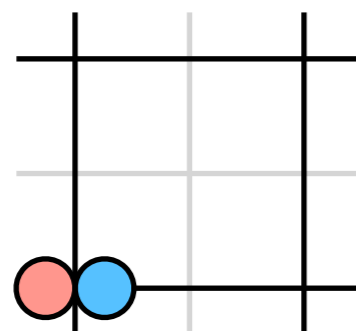


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Compare $\{BS\}$ and $\{AI\}$

- $\{BS\} \setminus \{AI\}$: subtraction of two sets

poor mathematical structure. like vector-bundle classification.

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- $\{BS\} / \{AI\}$: quotient of Abelian groups $\{BS\} < \{AI\}$

symmetry indicators: stable topology like K-theory.

need to allow “**negative integers**” in $\{BS\}$, $\{AI\}$

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- $\{BS\} \setminus \{AI\}$: subtraction of two sets

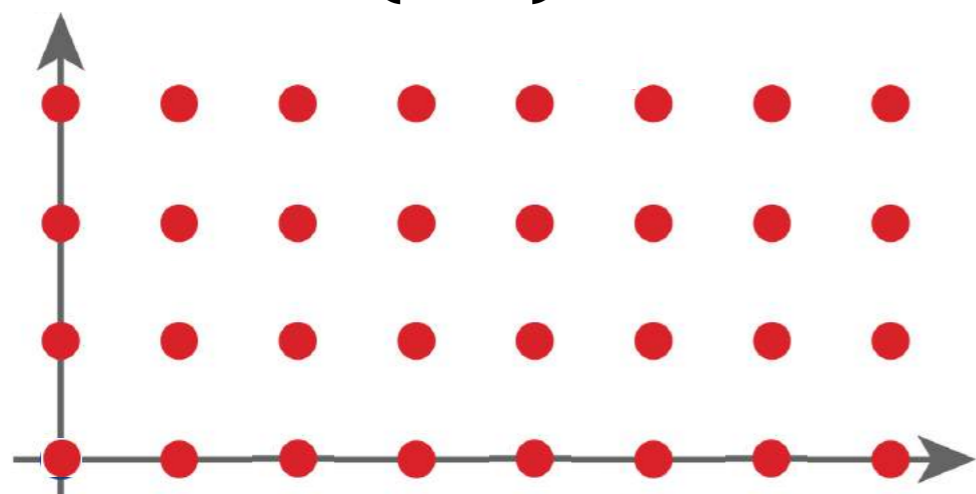
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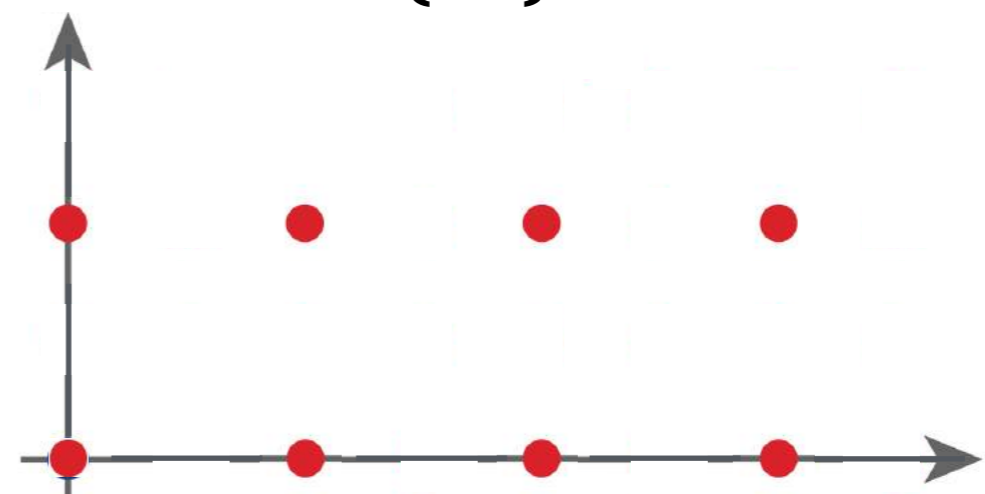
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lattice of $\{BS\}$



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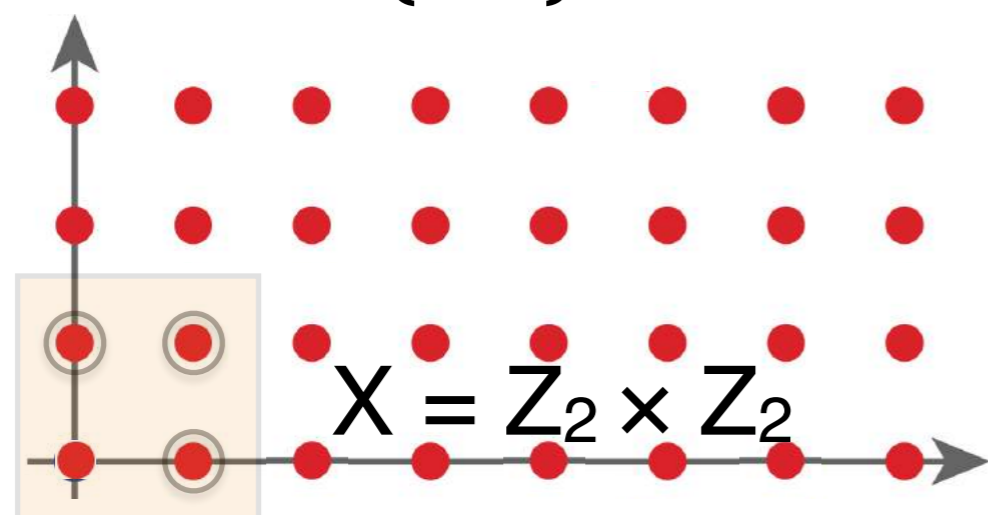
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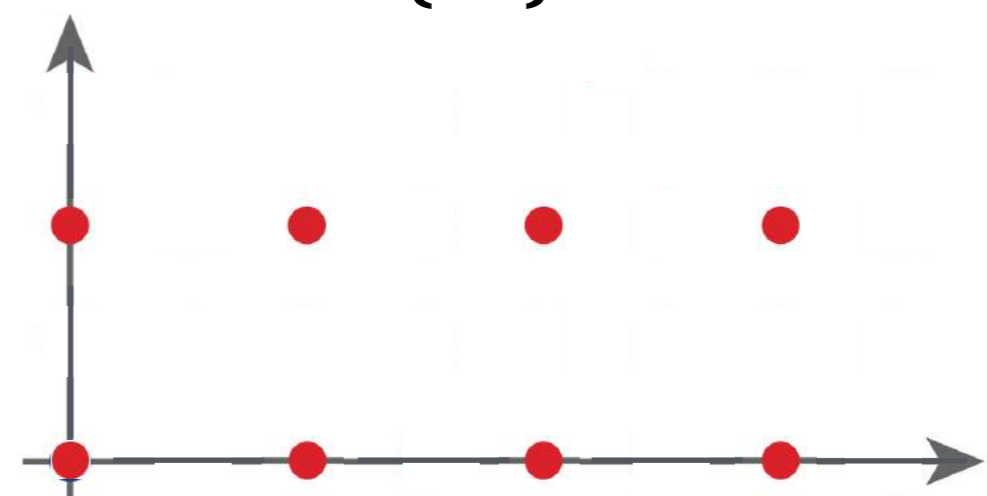
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lattice of $\{BS\}$



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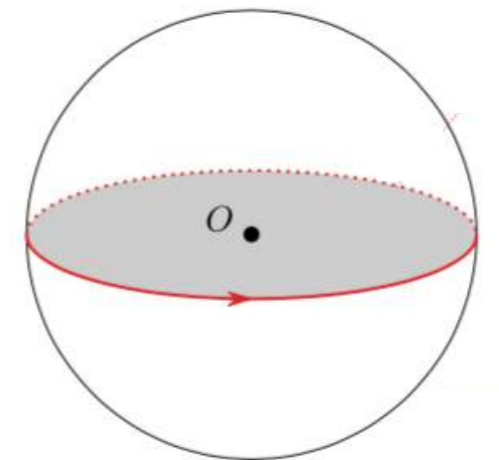
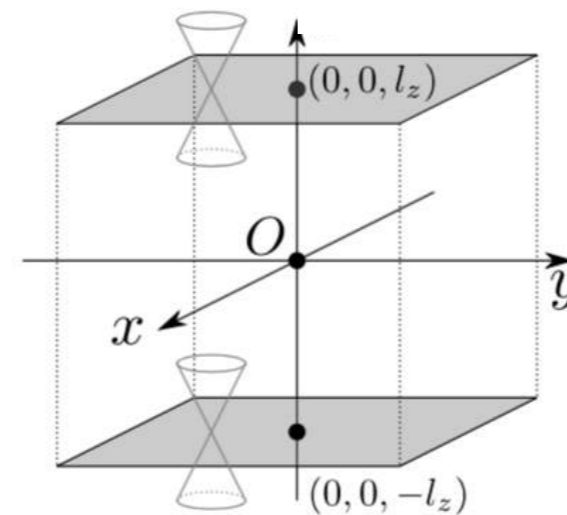
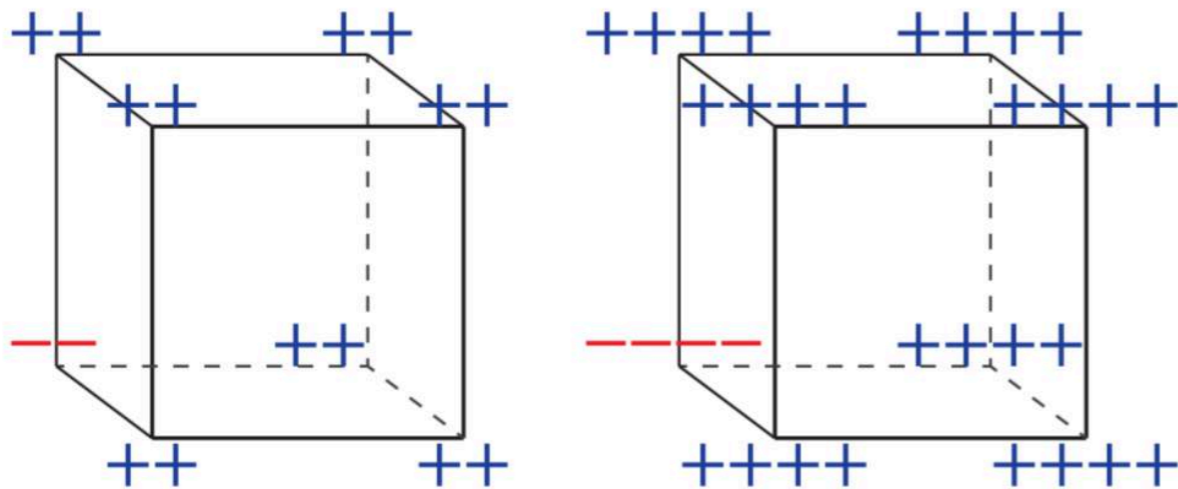
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Symmetry indicator for inversion & TRS with SOC in 3D

$$X = \mathbb{Z}_2 \times \mathbb{Z}_2 \times \mathbb{Z}_2 \times \mathbb{Z}_4$$

Sum of inversion parities

$$\kappa_1 \equiv \frac{1}{4} \sum_{K \in \text{TRIMs}} (n_K^+ - n_K^-) \in \mathbb{Z}.$$



Po-Vishwanath-Watanabe, Nat. Commun. (2017)

Chen Fang & Liang Fu, arXiv:1709.01929

Khalaf-Po-Vsiwanath-Watanabe, PRX (2018)

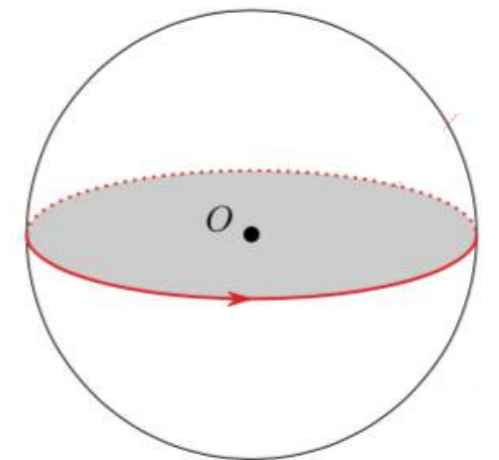
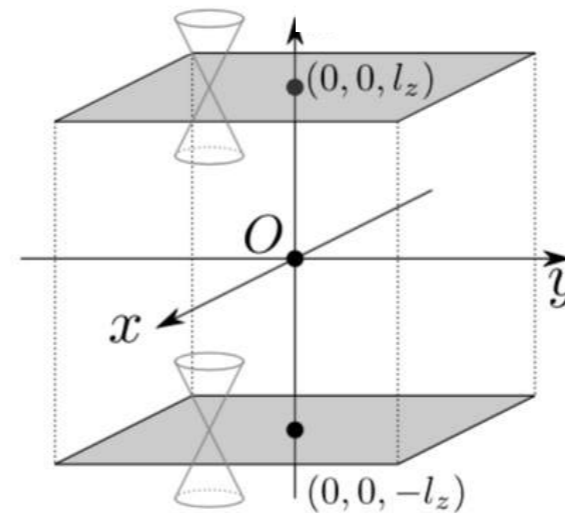
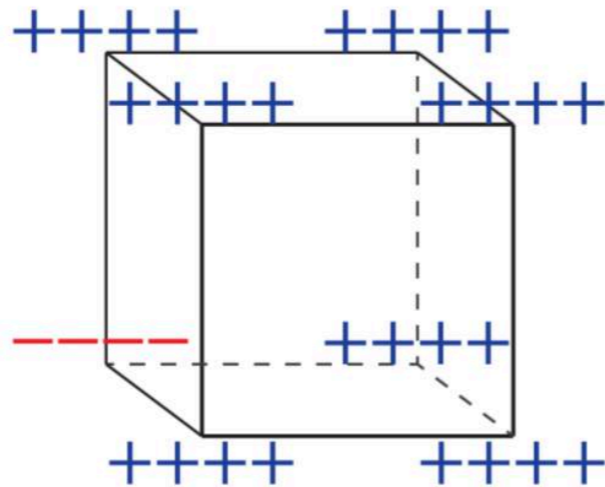
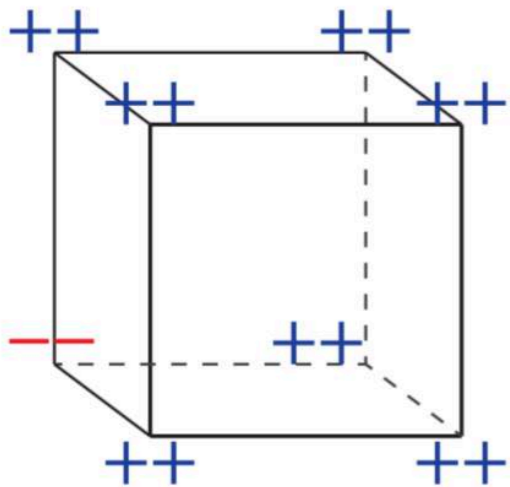
Symmetry indicator for inversion & TRS with SOC in 3D

$$X = \mathbb{Z}_2 \times \mathbb{Z}_2 \times \mathbb{Z}_2 \times \mathbb{Z}_4$$

weak TI

Sum of inversion parities

$$\kappa_1 \equiv \frac{1}{4} \sum_{K \in \text{TRIMs}} (n_K^+ - n_K^-) \in \mathbb{Z}.$$



Po-Vishwanath-Watanabe, Nat. Commun. (2017)

Chen Fang & Liang Fu, arXiv:1709.01929

Khalaf-Po-Vsiwanath-Watanabe, PRX (2018)

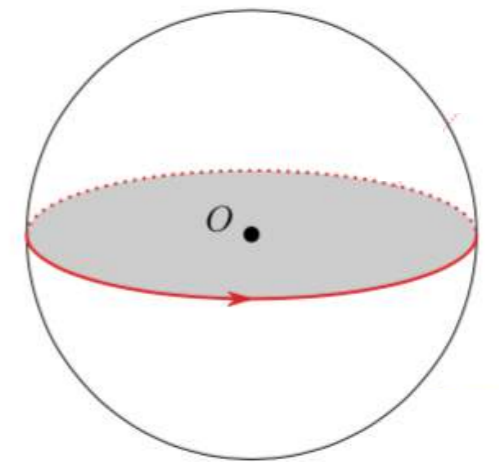
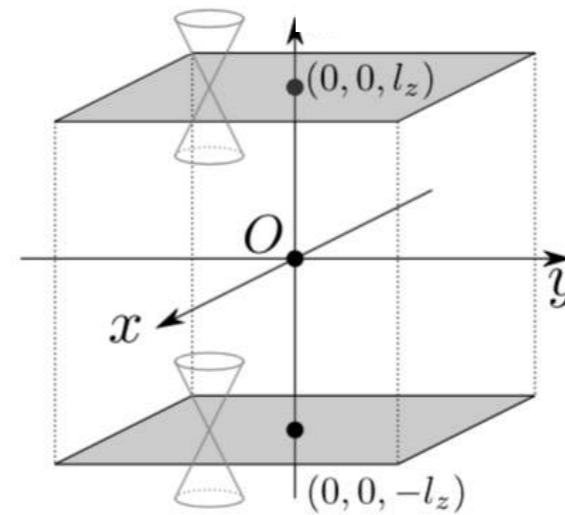
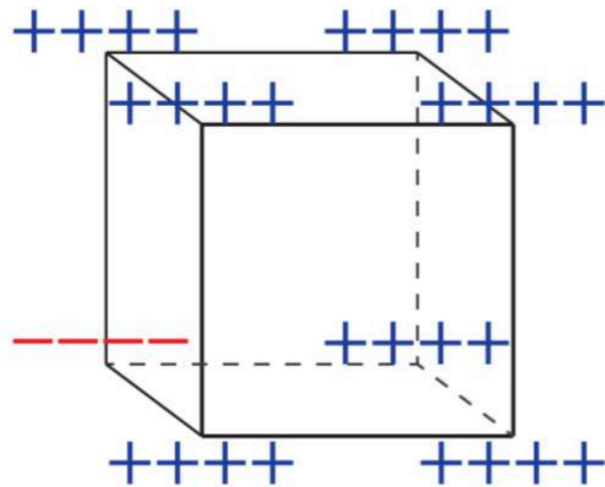
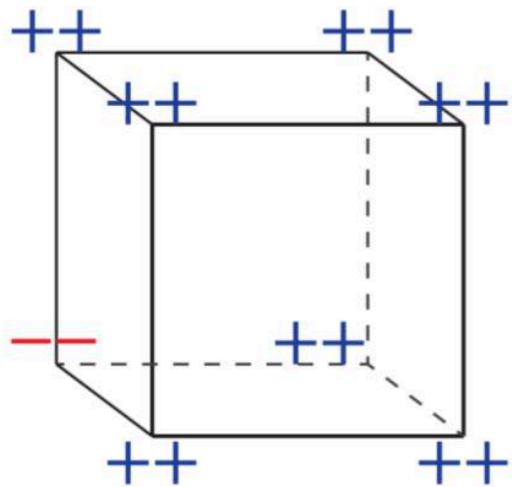
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weak TI strong TI + α

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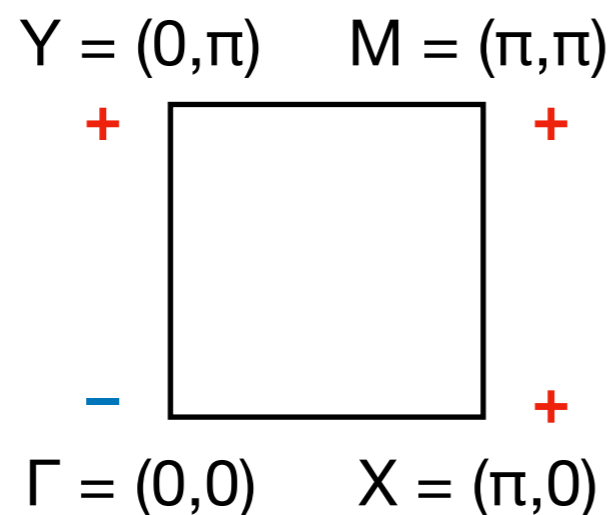
Po-Vishwanath-Watanabe, Nat. Commun. (2017)

Chen Fang & Liang Fu, arXiv:1709.01929

Khalaf-Po-Vsiwanath-Watanabe, PRX (2018)

Symmetry indicator for rotation symmetric systems in 2D

- n -fold rotation \rightarrow Chern number $C \bmod n$



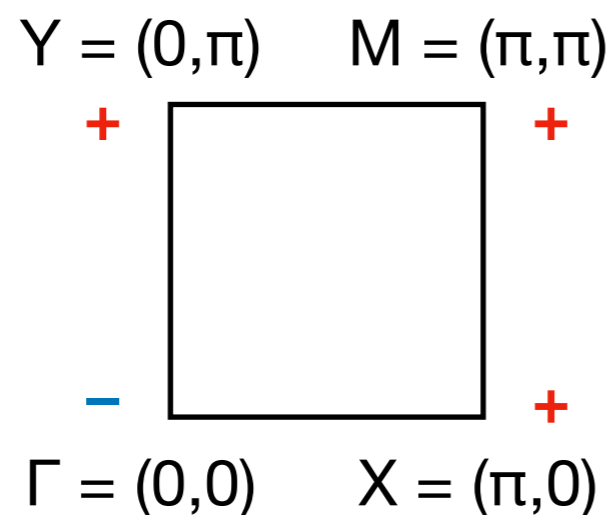
Fang-Gilbert-Bernevig PRB (2012)

$(-1)^C = \text{product of rotation eigenvalues}$

In our language, $X = \mathbb{Z}_n$

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Fang-Gilbert-Bernevig PRB (2012)

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In our language, $X = \mathbb{Z}_n$

- Extension to interacting systems using twisted boundary condition

Matsugatani-Ishiguro-Shiozaki-Watanabe PRL (2018)

$$(\hat{T}_x)^{L_x} = e^{-i\theta_x \hat{N}}, \quad (\hat{T}_y)^{L_y} = e^{-i\theta_y \hat{N}}$$

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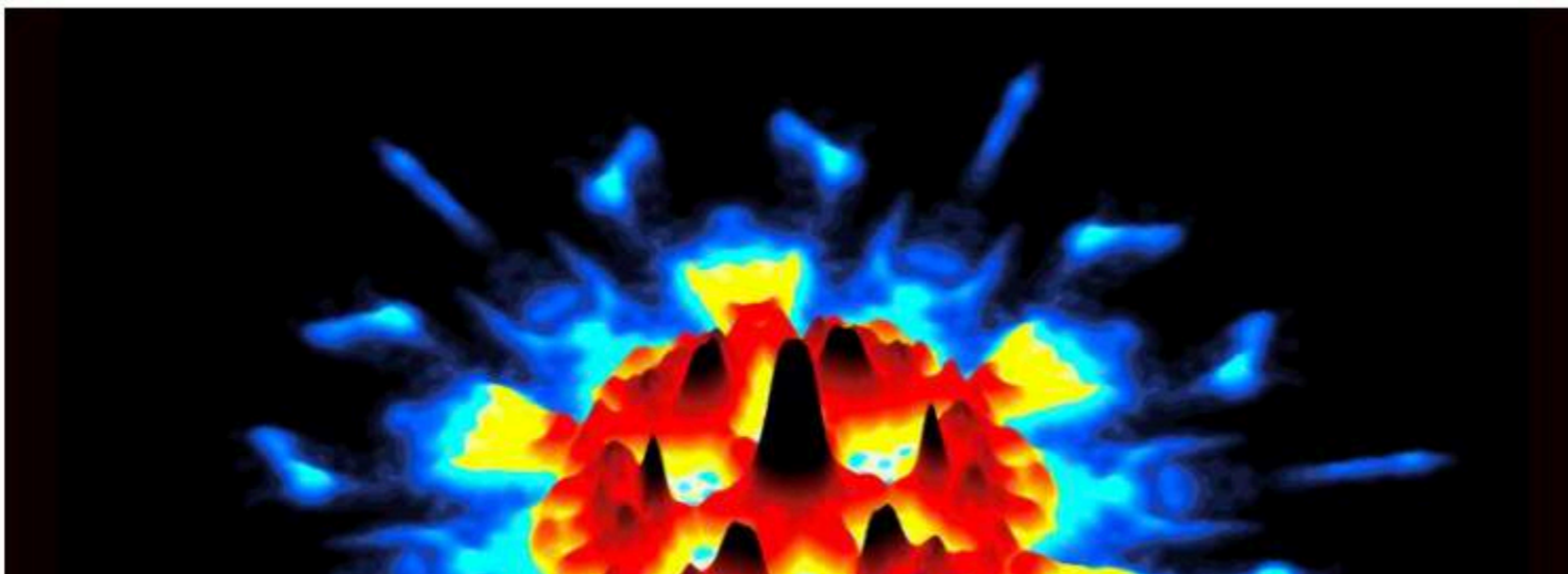
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Haul thrills physicists, who previously knew of just a few hundred of these peculiar materials.

Elizabeth Gibney



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 2. Higher-order topological insulators
 3. **Weyl semimetals**
 4. Fragile topology
 5. Topological superconductors

Symmetry indicator for TR breaking inversion symmetric system in 3D

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

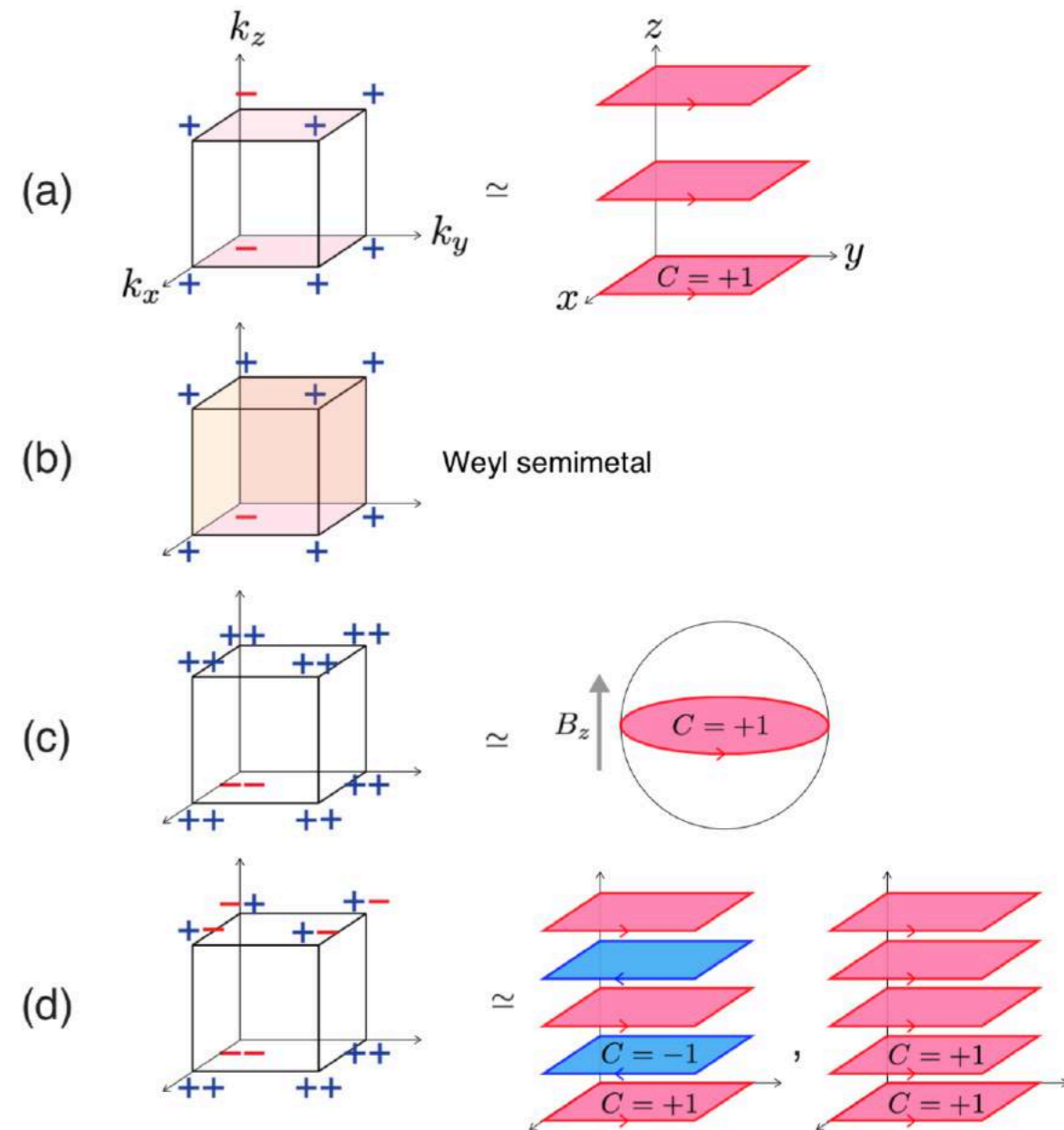
A. Turner, ..., A. Vishwanath (2010) Weyl SM

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

See also

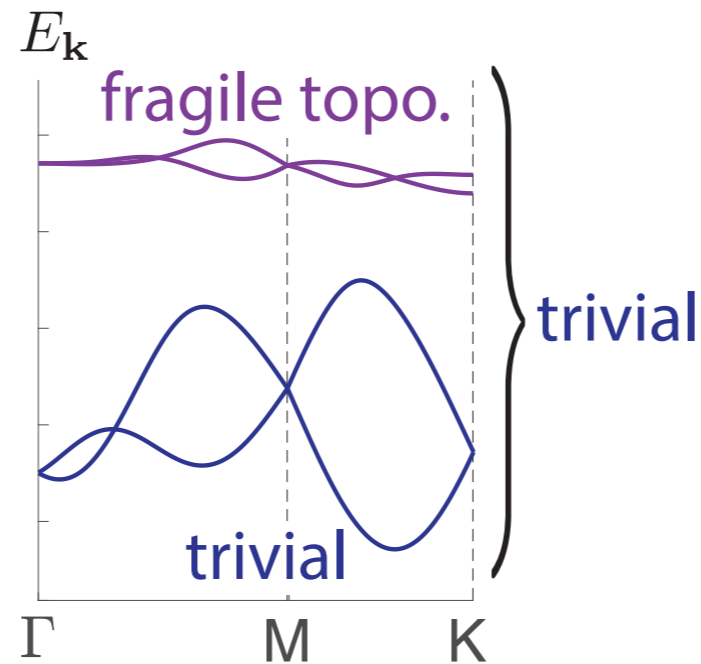
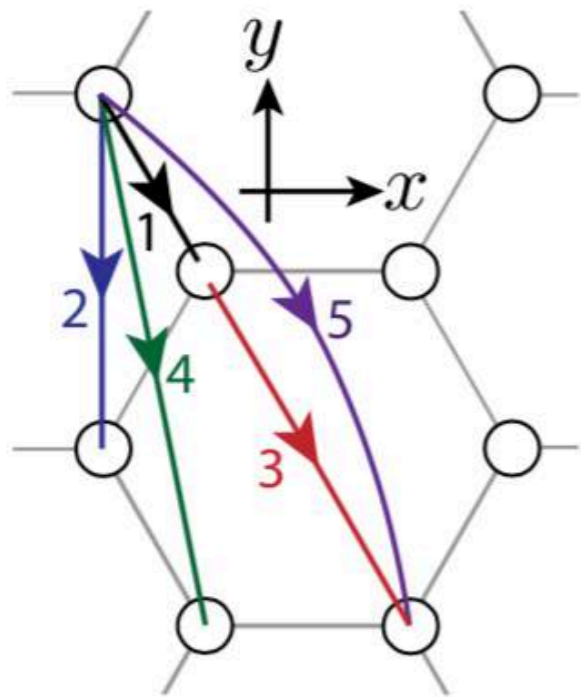
Song-Zhang-Fang PRX (2018)

for nodal semimetals in the absence of SOC

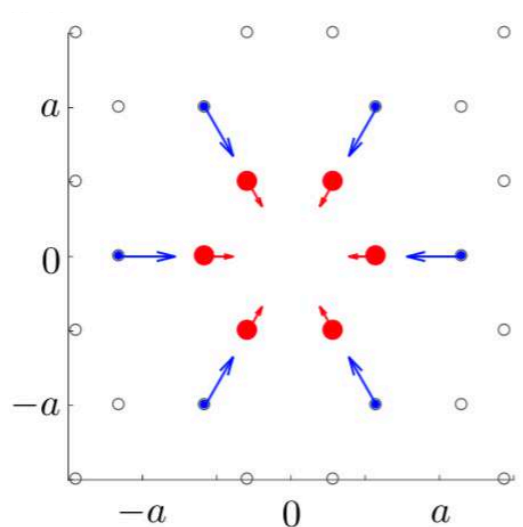


- Basics of symmetry indicators
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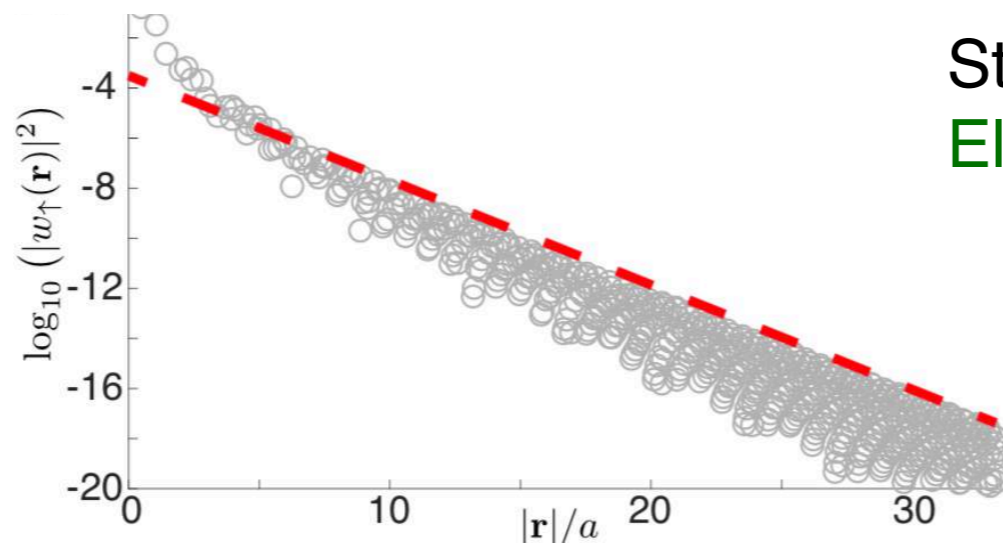
Honeycomb lattice with SOC



Po-Watanabe-Vishwanath PRL (2018)

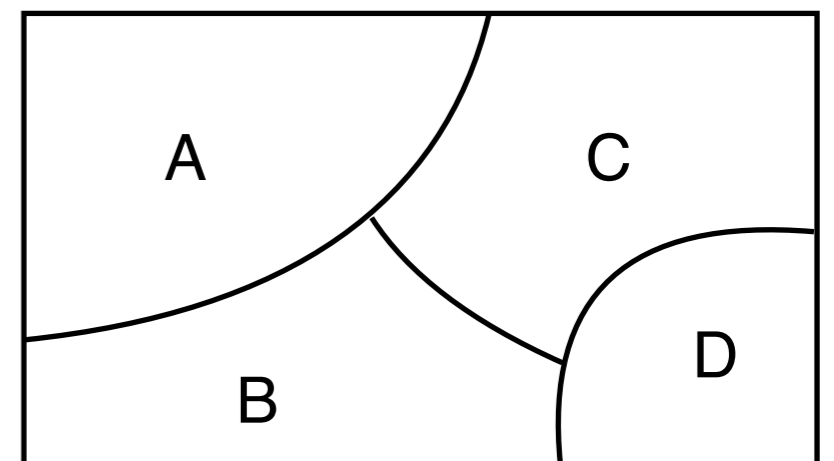


Wannier orbital

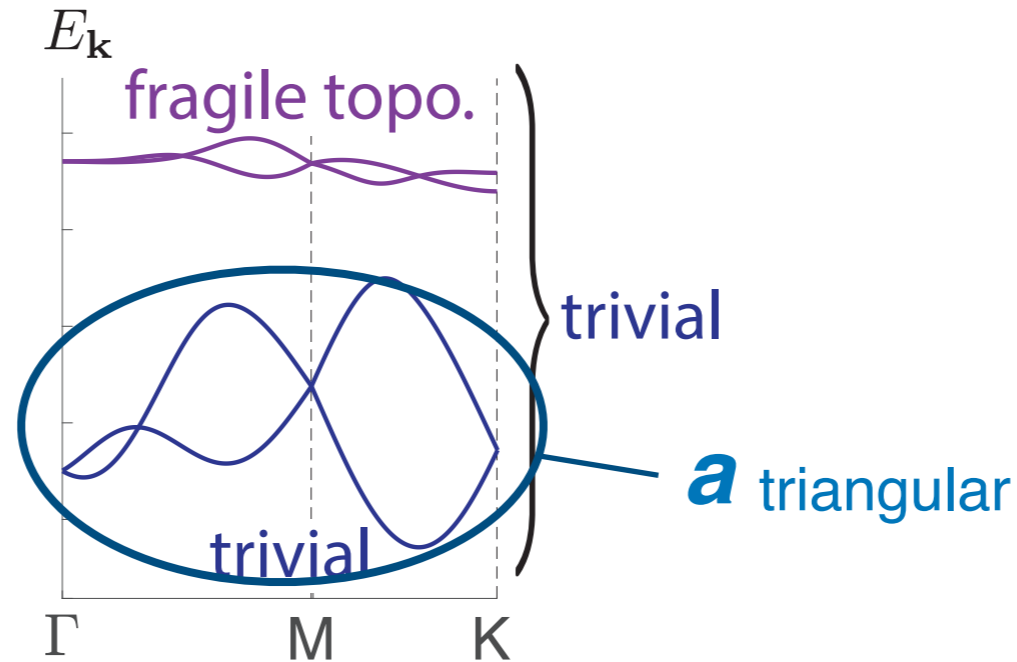
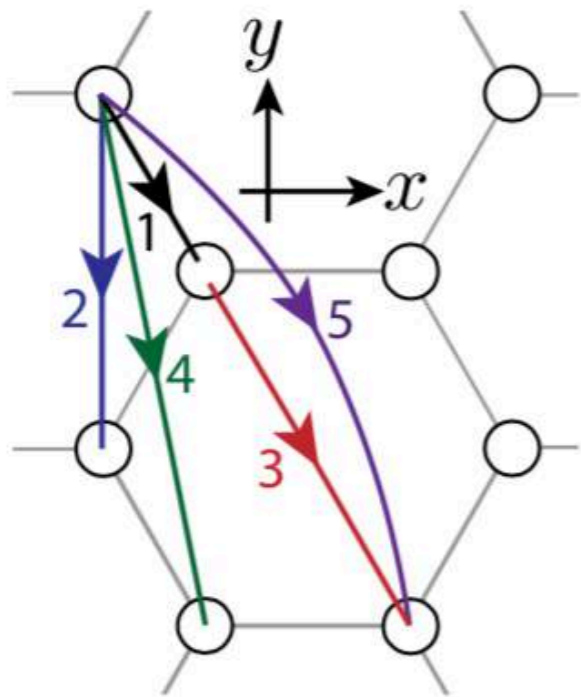


Exponential decay of Wannier

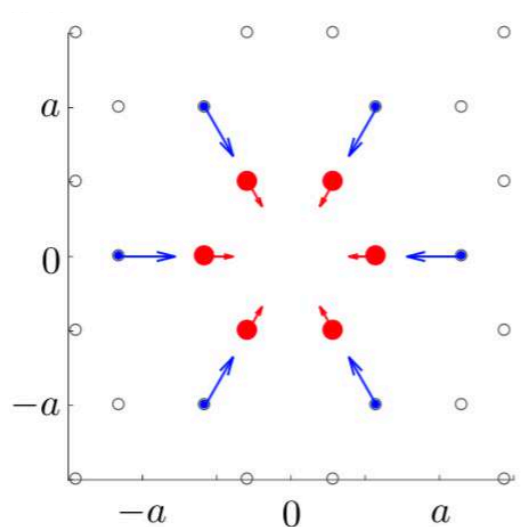
Stability against interaction:
Else-Po-Watanabe arXiv:1809.02128



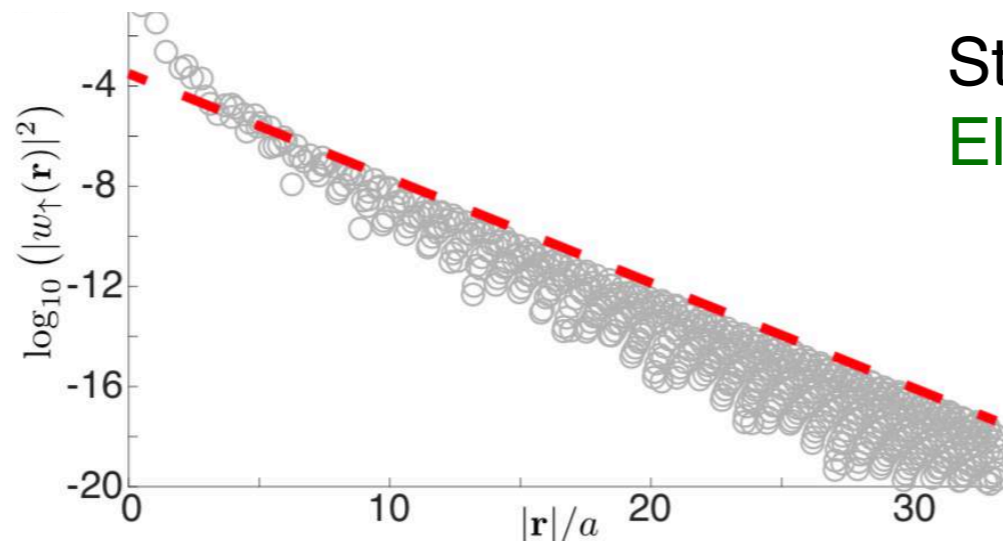
Honeycomb lattice with SOC



Po-Watanabe-Vishwanath PRL (2018)

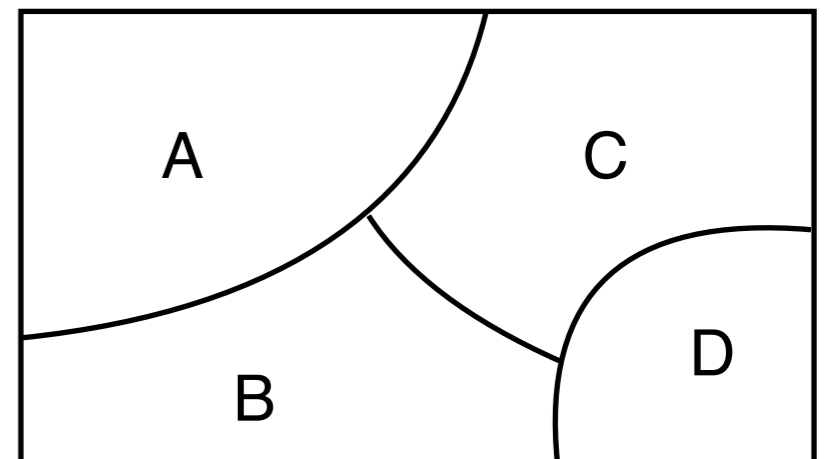


Wannier orbital

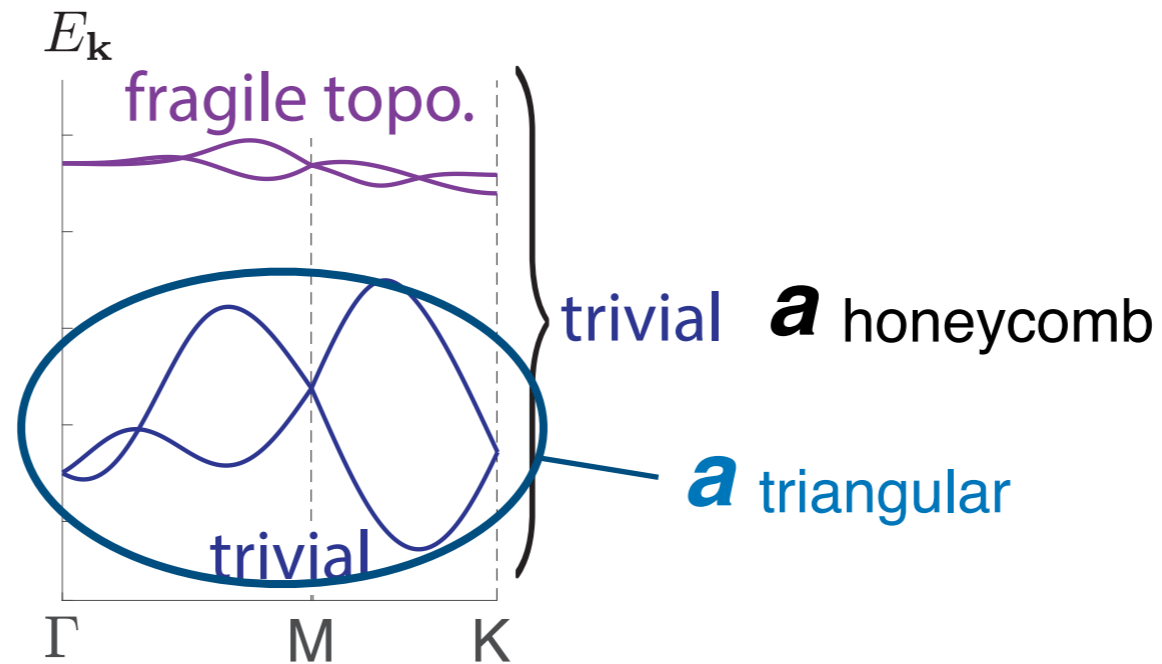
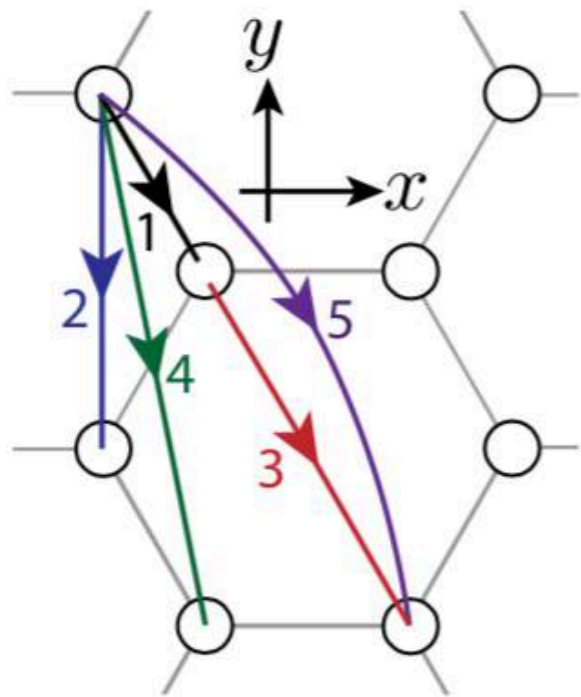


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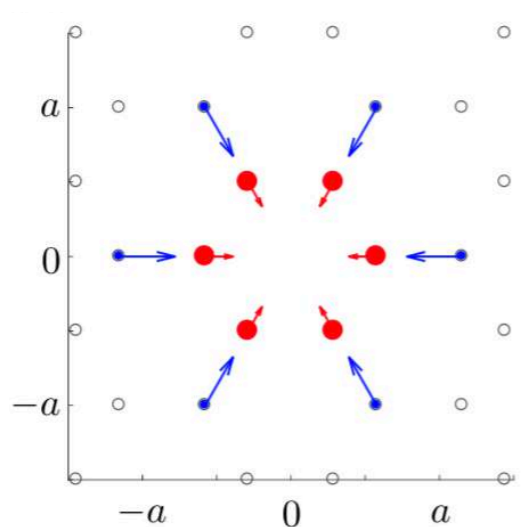
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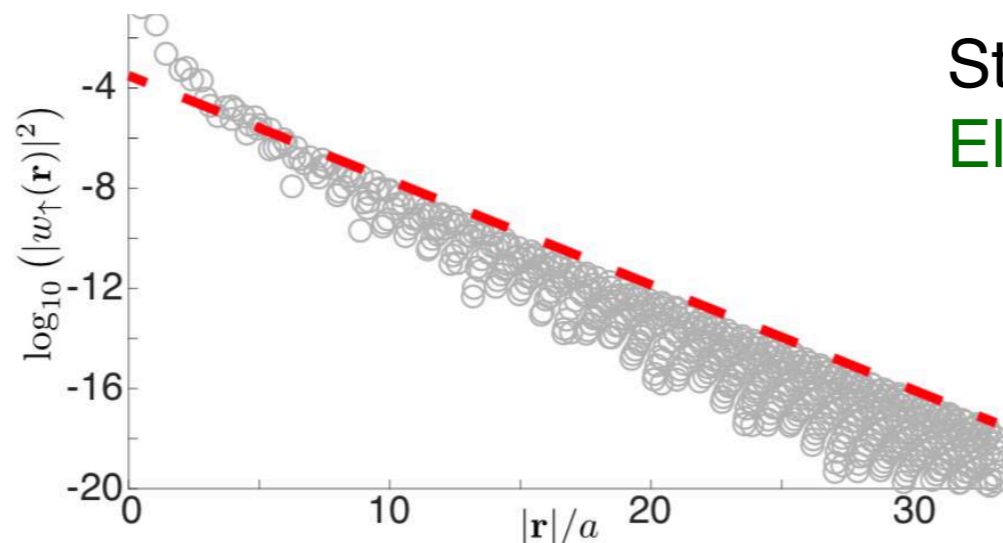
Honeycomb lattice with SOC



Po-Watanabe-Vishwanath PRL (2018)

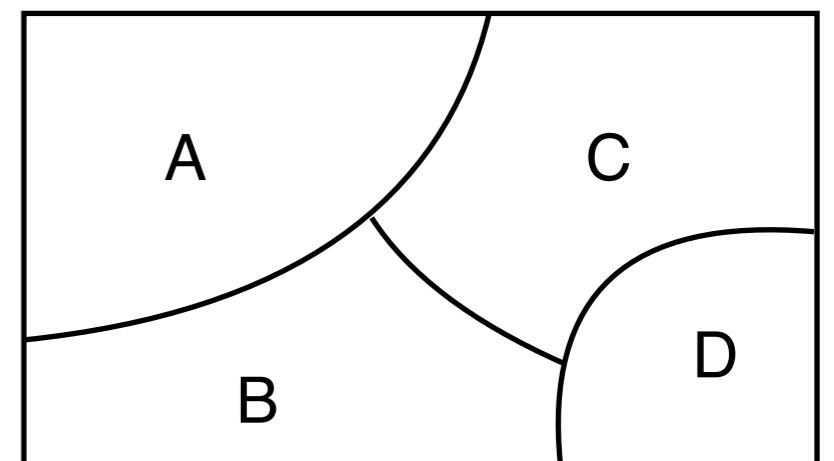


Wannier orbital

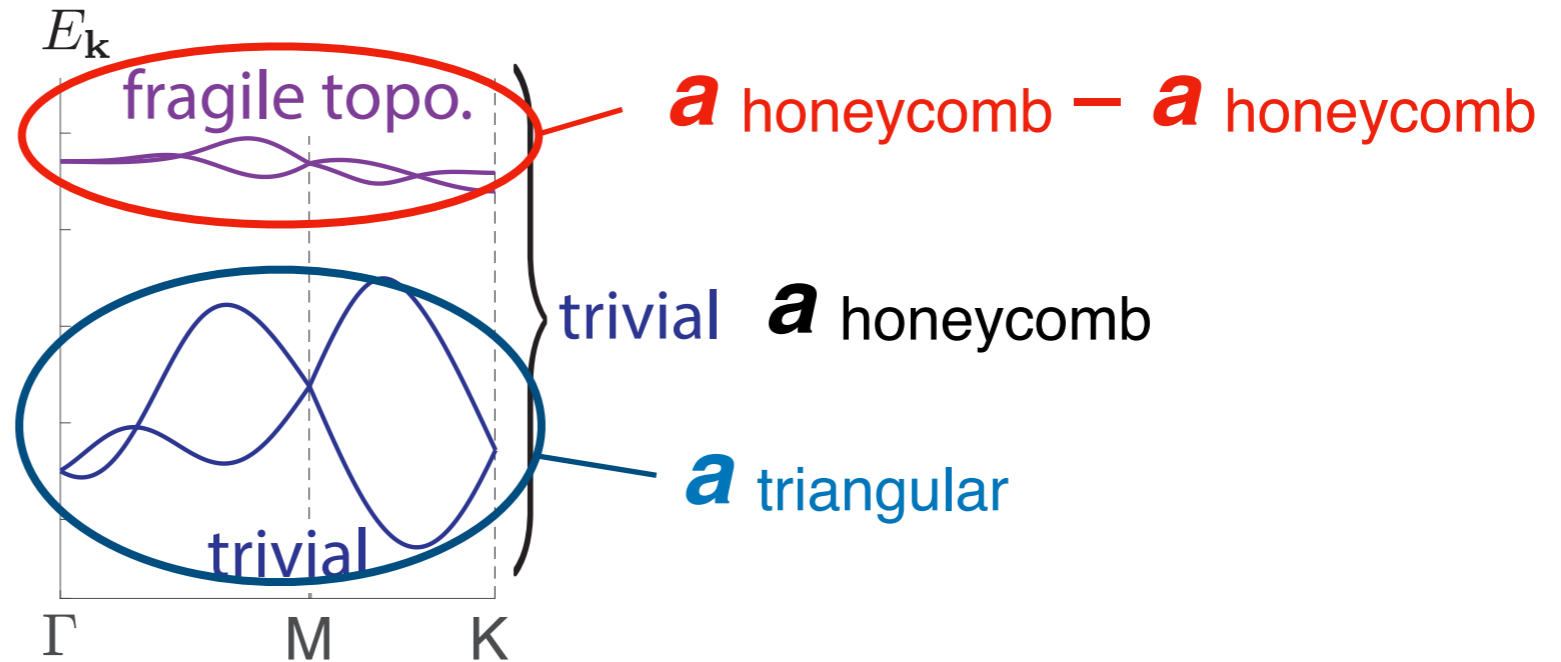
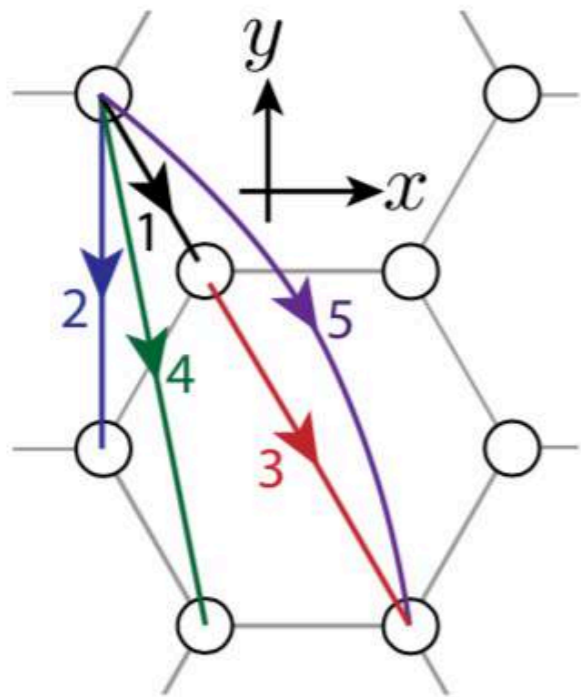


Exponential decay of Wannier

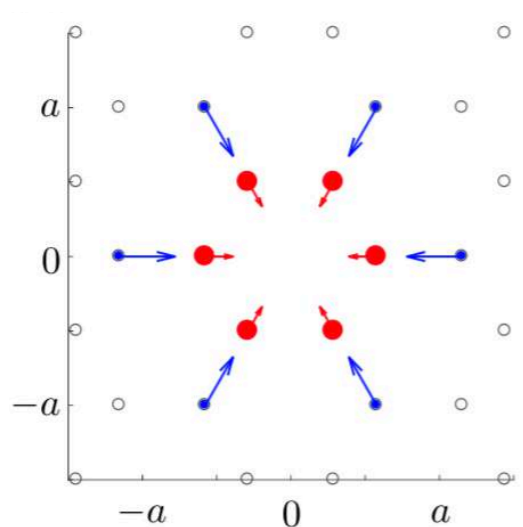
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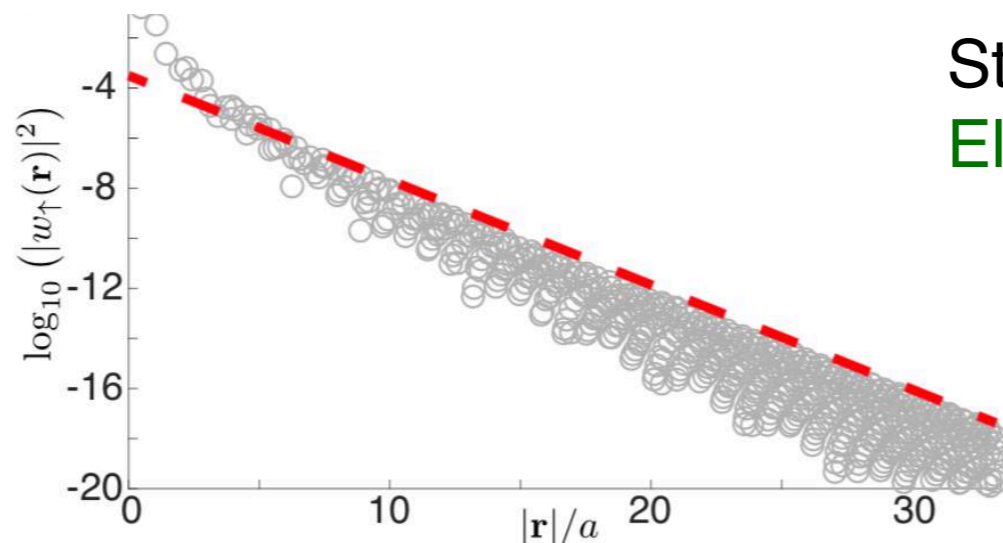
Honeycomb lattice with SOC



Po-Watanabe-Vishwanath PRL (2018)

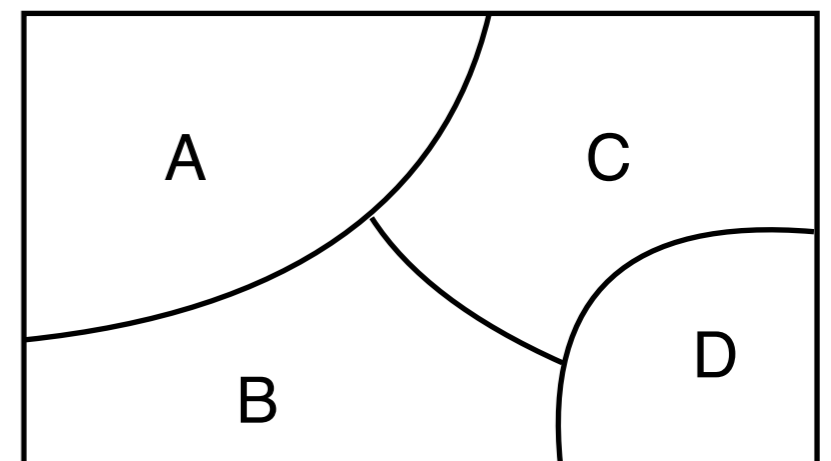


Wannier orbital



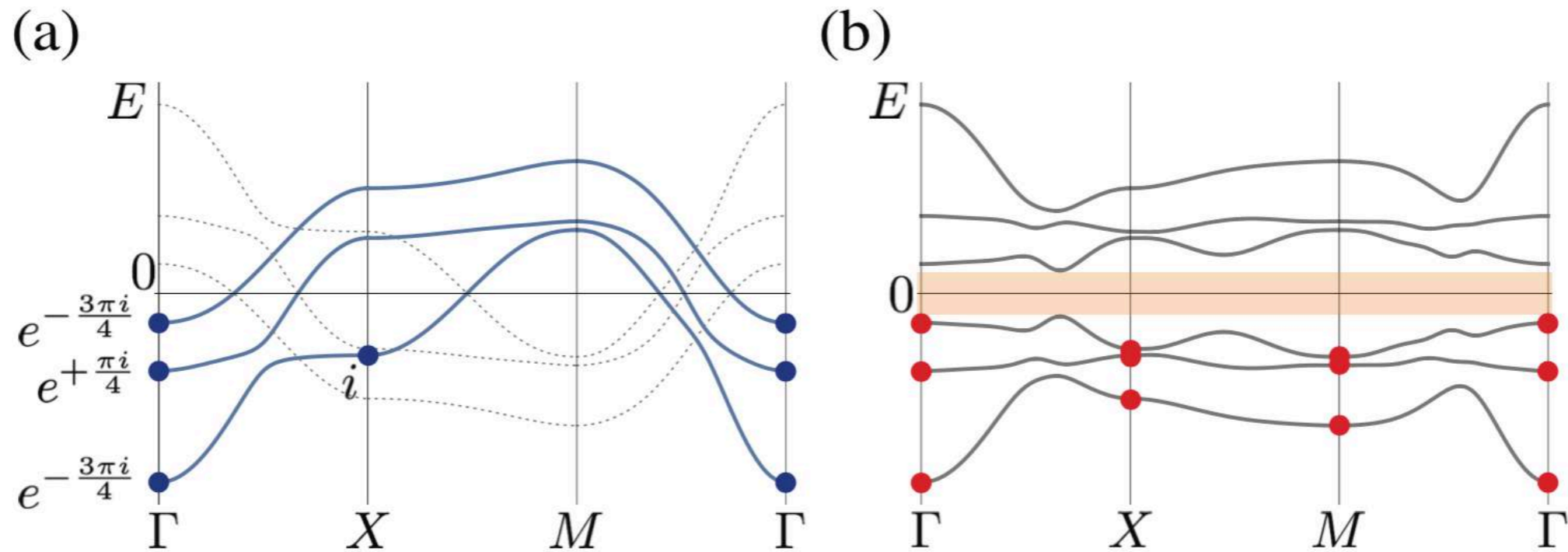
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- Basics of symmetry indicators
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Weak-coupling assumption



$$H_{\mathbf{k}}^{\text{BdG}} = \begin{pmatrix} H_{\mathbf{k}} & \Delta_{\mathbf{k}} \\ \Delta_{\mathbf{k}}^{\dagger} & -H_{-\mathbf{k}}^* \end{pmatrix}$$

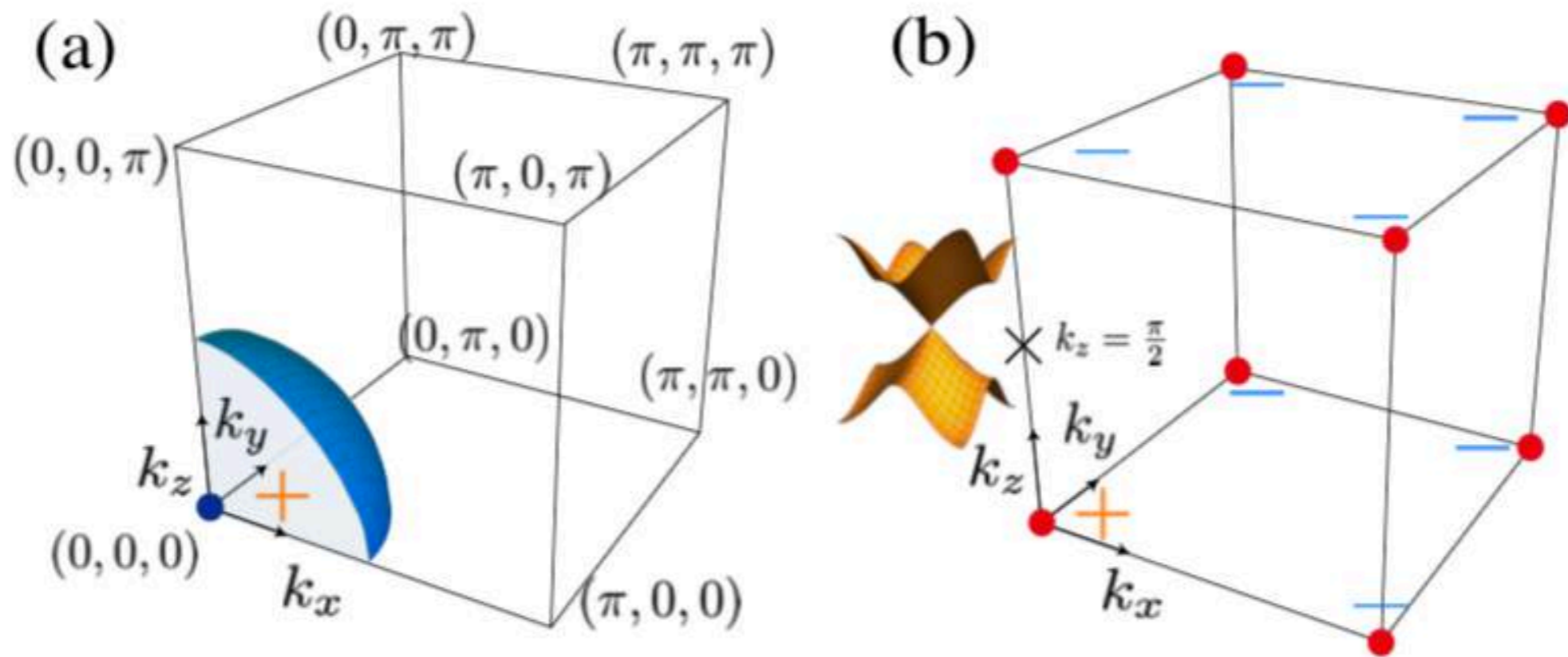
$$\begin{aligned} (n_{\mathbf{k}}^{\alpha})^{\text{BdG}} &= n_{\mathbf{k}}^{\alpha} \Big|_{\text{occ.}} + n_{-\mathbf{k}}^{f_{-\mathbf{k}}(\alpha)} \Big|_{\text{unocc.}} \\ &= (n_{\mathbf{k}}^{\alpha} - n_{-\mathbf{k}}^{f_{-\mathbf{k}}(\alpha)}) \Big|_{\text{occ.}} + n_{-\mathbf{k}}^{f_{-\mathbf{k}}(\alpha)} \Big|_{\text{all bands}} \end{aligned}$$

$$U_{\mathbf{k}}^{\text{BdG}}(g) = \begin{pmatrix} U_{\mathbf{k}}(g) & 0 \\ 0 & \chi_g U_{-\mathbf{k}}(g)^* \end{pmatrix}$$

We can extract indicators for SCs from the band structure in the normal phase!

$p+ip$ SC with nodes

(SC version of Weyl semimetal)



$$H_{\mathbf{k}} = t(3 - \cos k_x - \cos k_y - \cos k_z) - \mu,$$

$$\Delta_{\mathbf{k}} = \Delta(\sin k_x + i \sin k_y).$$

Summary

- Extract band topology by comparing {BS} and {AI}
Nat. Commun. (2017) Sci. Adv. (2018)
- Applications include
 1. Conventional topological insulators (Chern, Z2 TI, etc) PRL (2018)
 2. Higher-order topological insulators PRX (2018)
 3. Weyl semimetals
 4. Fragile topology PRL (2018), arXiv:1809.02128
 5. Topological superconductors PRB (2018), arXiv:1811.08712

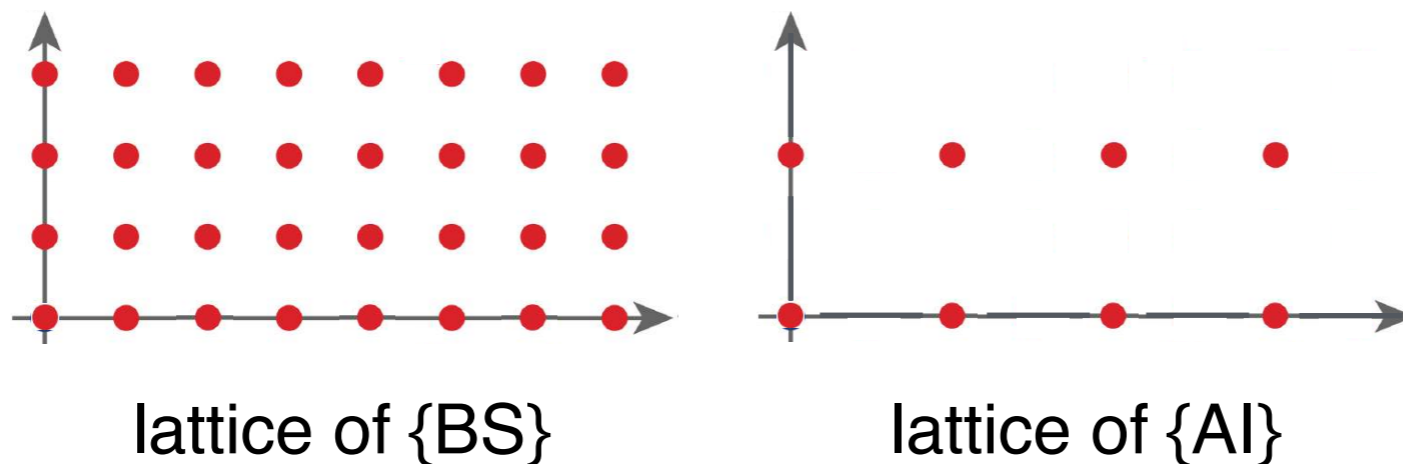
A useful fact

$$dBS = dAI$$

Po-Vishwanath-Watanabe
Nat. Commun. (2017)

$$\{BS\} = \{\mathbf{b} = \{n_k^\alpha\} \mid \text{satisfying compatibility rels.}\} \subset \mathbb{Z}^{dBS}$$

$$\{AI\} = \{\mathbf{a} = \{n_k^\alpha\} \mid \text{corresponding to AI}\} \subset \mathbb{Z}^{dAI}$$



$$\begin{pmatrix} + \\ + \\ + \\ - \end{pmatrix} = \mathbf{1/2} \left[\begin{pmatrix} + \\ + \\ + \\ + \end{pmatrix} + \begin{pmatrix} + \\ + \\ - \\ - \end{pmatrix} + \begin{pmatrix} + \\ - \\ + \\ - \end{pmatrix} - \begin{pmatrix} + \\ - \\ - \\ + \end{pmatrix} \right]$$

$\mathbf{b} \qquad \mathbf{a}_1 \qquad \mathbf{a}_2 \qquad \mathbf{a}_3 \qquad \mathbf{a}_4$

We do not have to solve compatibility relations to find out {BS}!