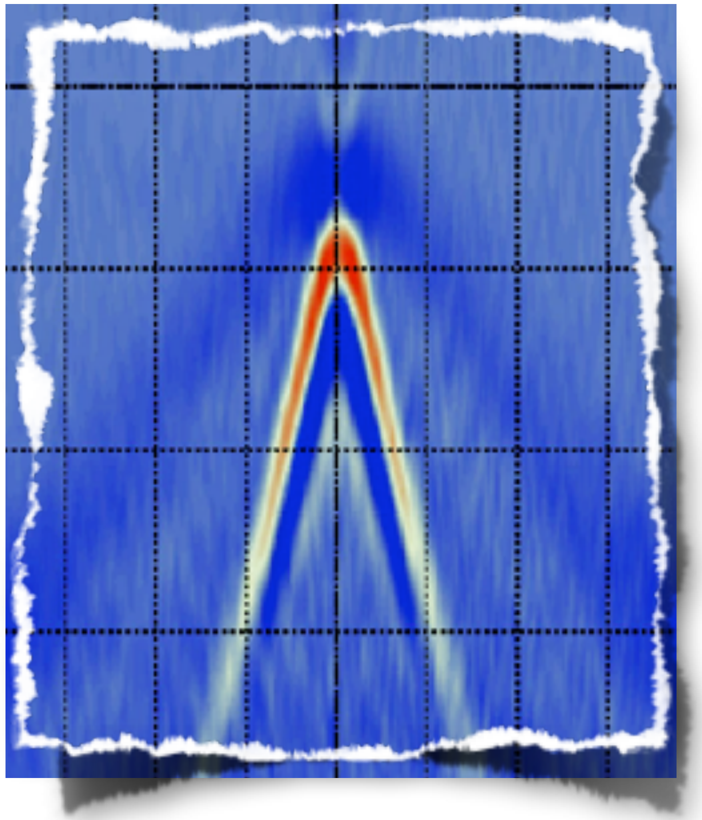
Topological Order in Insulators

Pedestrian introduction *via* simple models

D. Carpentier, M. Fruchart, K. Gawędzki
(Ecole Normale Supérieure de Lyon)



Journées de Physique Mathématique LYON
11 - 13 september 2013

Topological Order in Insulators

- How do we describe bands in an insulator

- Chern Topological Order (Quantum Hall Effect)

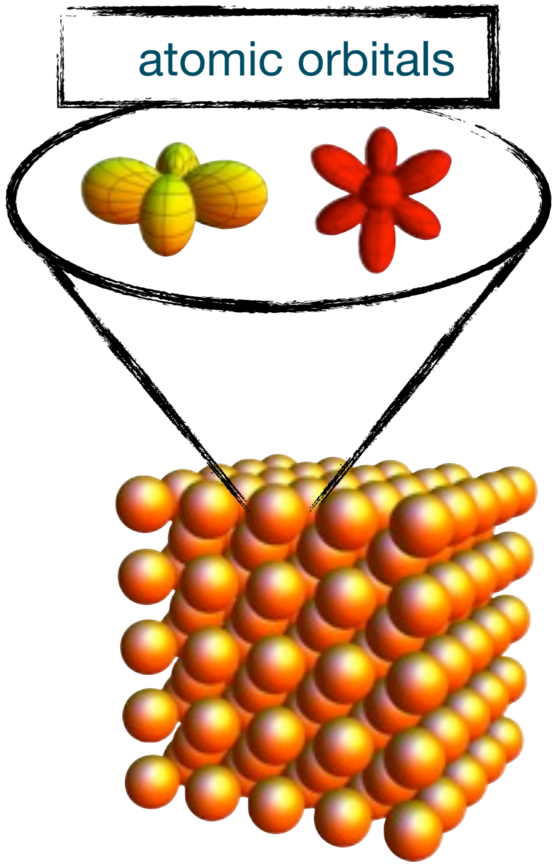
  on simple 2 bands models

- Z_2 Topological Order

  on simple 4 bands models

Purpose : illustrate topological orders as an obstruction using simple models

Filled Bands in an Insulator



electrons on a lattice

- Number of bands (orbitals, spin, sub-lattices) : N ⇒ NxN Hamiltonian H
- State of electrons satisfy $H\psi^{\alpha}_{\mathbf{k}} = E^{\alpha}_{\mathbf{k}}\ \psi^{\alpha}_{\mathbf{k}}$ for $\alpha = 1, \cdots, N$

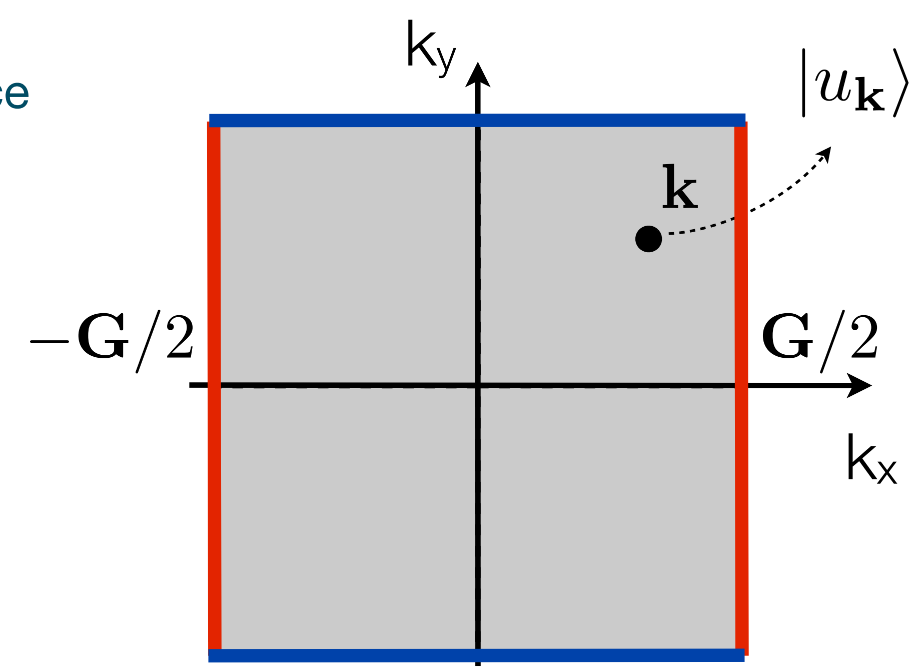
  wavefunction ($\psi^{\alpha}_{\mathbf{k}}$) energy ($E^{\alpha}_{\mathbf{k}}$)

- Periodicity of lattice ⇒ Bloch wavefunctions

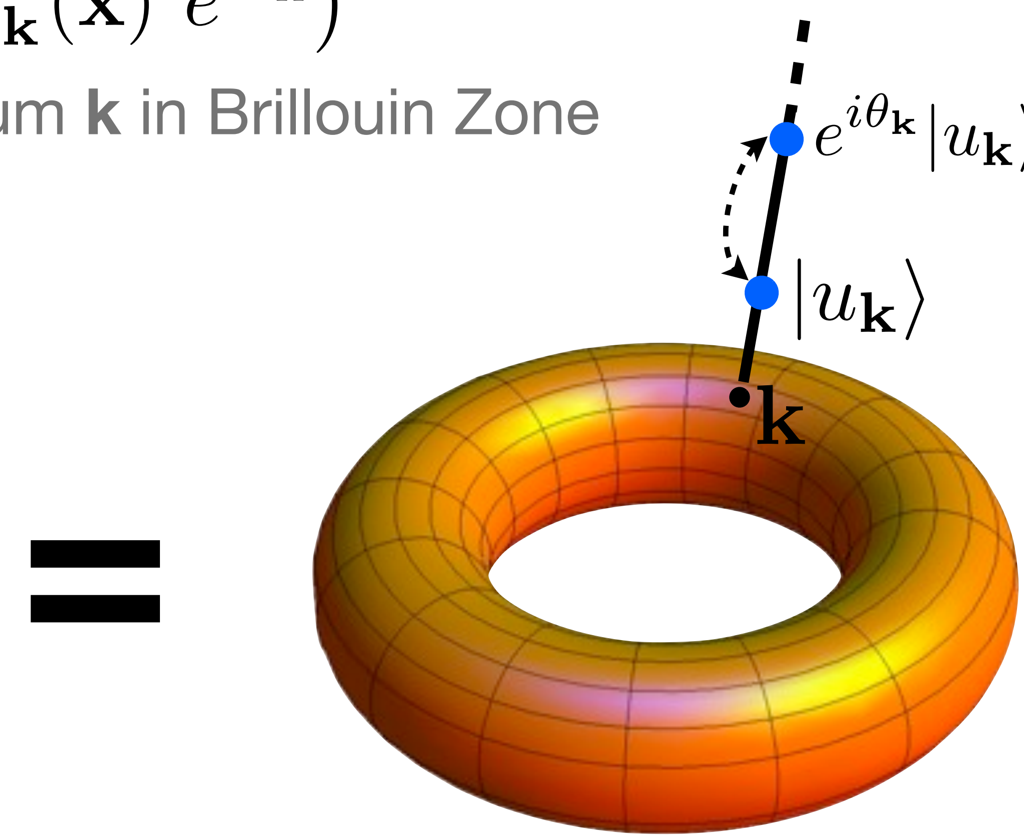
$$\psi^{\alpha}_{\mathbf{k}}(\mathbf{x}) = e^{i\mathbf{k}.\mathbf{x}}.\left(u^{\alpha}_{\mathbf{k}}(\mathbf{x})\ e^{i\theta_{\mathbf{k}}}\right)$$

indexed by momentum **k** in Brillouin Zone

Quantum Mechanics : arbitrary phase



Brillouin Zone

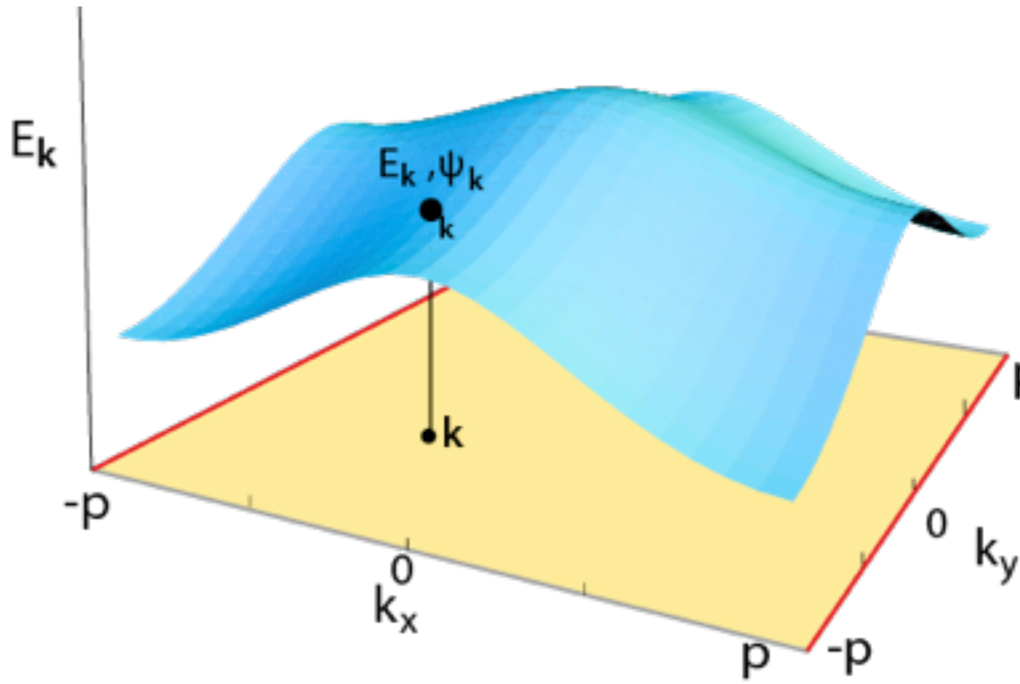


Filled Bands in an Insulator

$\alpha = 1, \cdots, N$

- Bloch wavefunctions $H\psi_{\mathbf{k}}^{\alpha} = E_{\mathbf{k}}^{\alpha}\ \psi_{\mathbf{k}}^{\alpha}\ , \psi_{\mathbf{k}}^{\alpha}(\mathbf{x}) = e^{i\mathbf{k}.\mathbf{x}}.\ \left(u_{\mathbf{k}}^{\alpha}(\mathbf{x})\ e^{i\theta_{\mathbf{k}}}\right)$

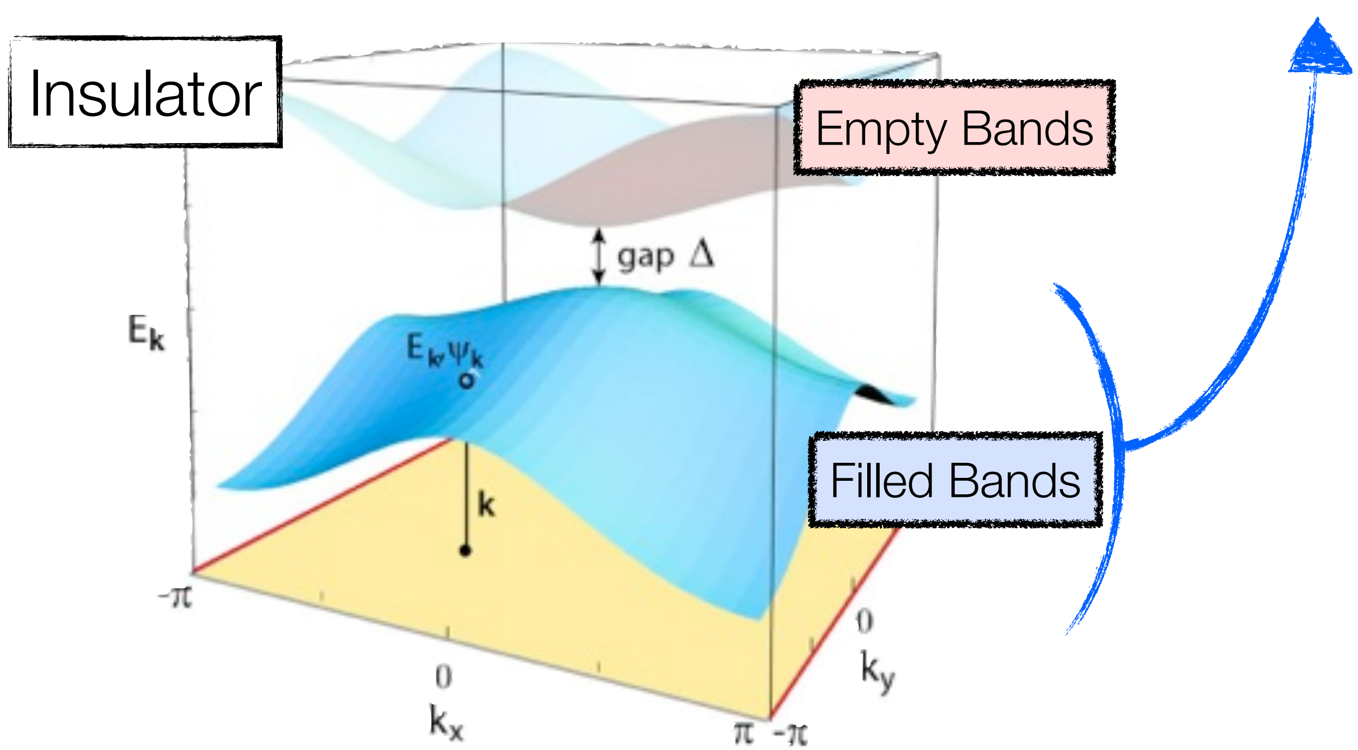
- $E_{\mathbf{k}}^{\alpha}$ defines an energy band :

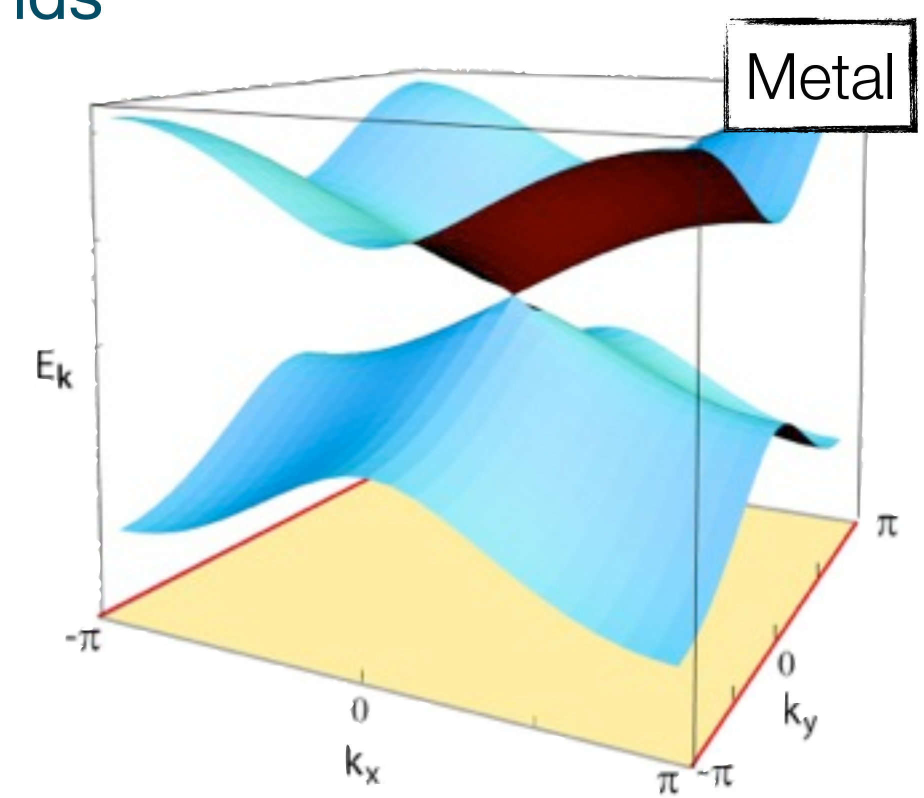


for each α

Brillouin Zone

- Insulator : well defined ensemble of occupied bands





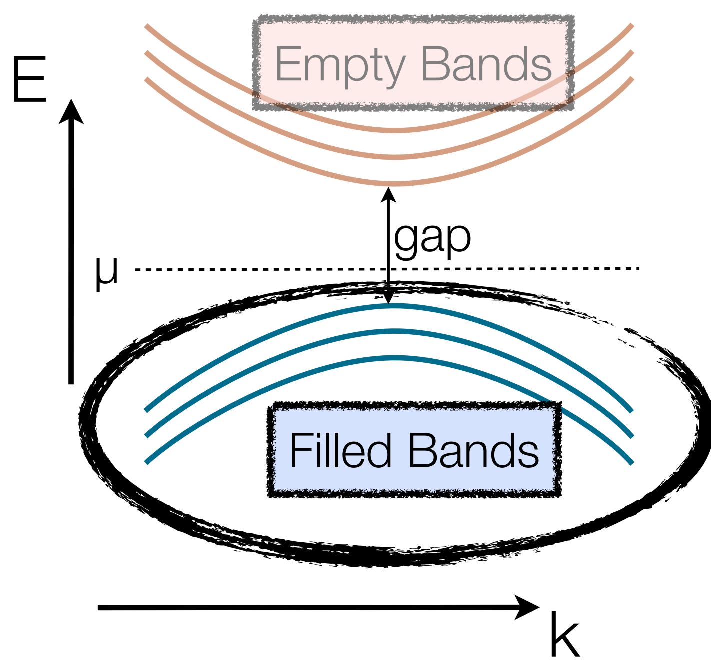
Filled Bands in an Insulator

- Insulator : ground state characterized by ensemble of filled bands
- ensemble of filled bands (valence Bloch bundle) : well defined (robust) object

Filled Band ⇔ Ensemble of states $|u_{\mathbf{k}}\rangle$ over the Brillouin Zone

⇕

Fiber Bundle over the Brillouin Torus



➡ Topological properties of this 'valence Bloch bundle' ?

(total ensemble of bands is always trivial)

Topological Insulator ⇔ non trivial topology of valence Bloch bundle

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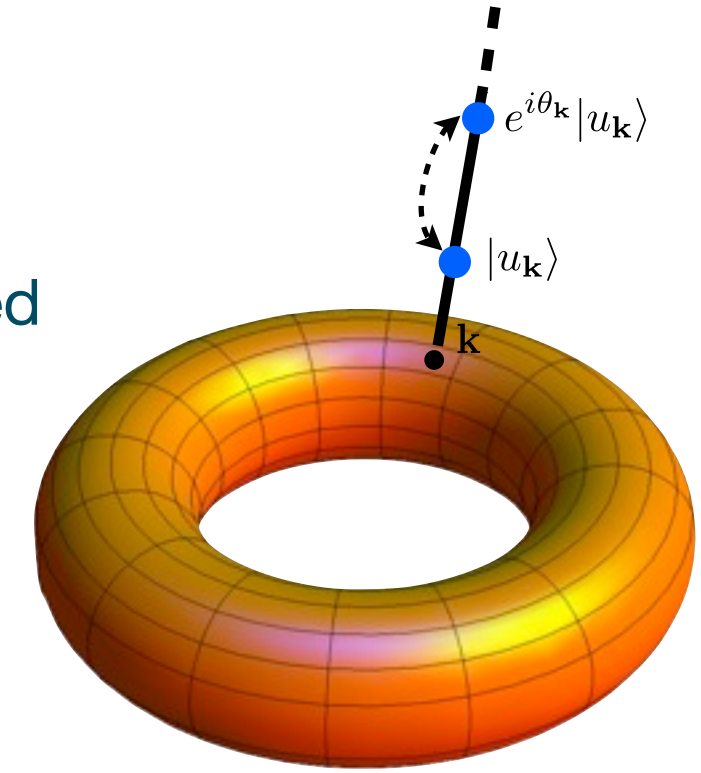

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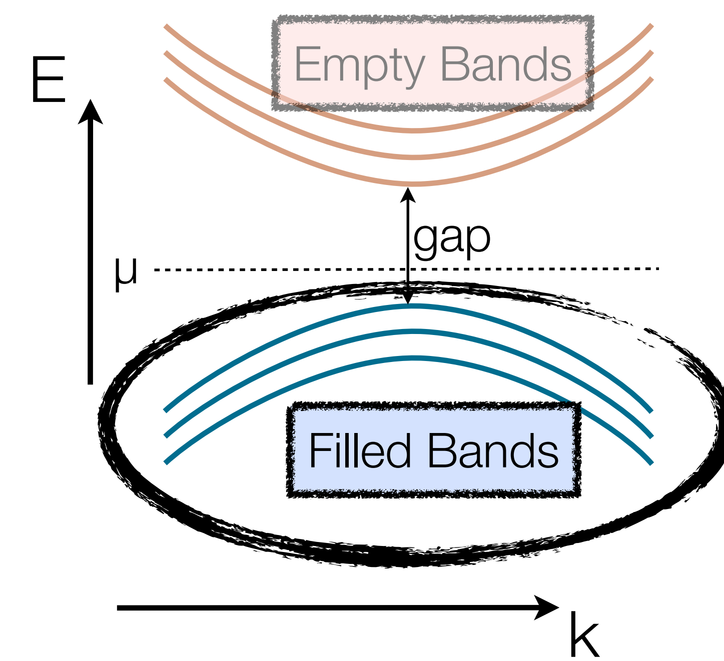

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Topological Insulator ⇔ non trivial topology of valence Bloch bundle

Topological Order in Insulators

- Chern Topological Order (Quantum Hall Effect) :
  - breaking of time-reversal (e.g. Magnetic Field)
  - no Spin (a single Chern number per band)
  - only d=2
- Z_2 Topological Order :
  - spin dependent bands (S=½)
  - time reversal symmetry (e.g. spin-orbit interaction)
  - induced by strong spin-orbit (material property)
  - occurs in d=2 and d=3

Here : focus on bulk topological order

Thouless *et al.* (1982)
Haldane (1985)

C.L.Kane and E.J.Mele PRL **95** (2005)
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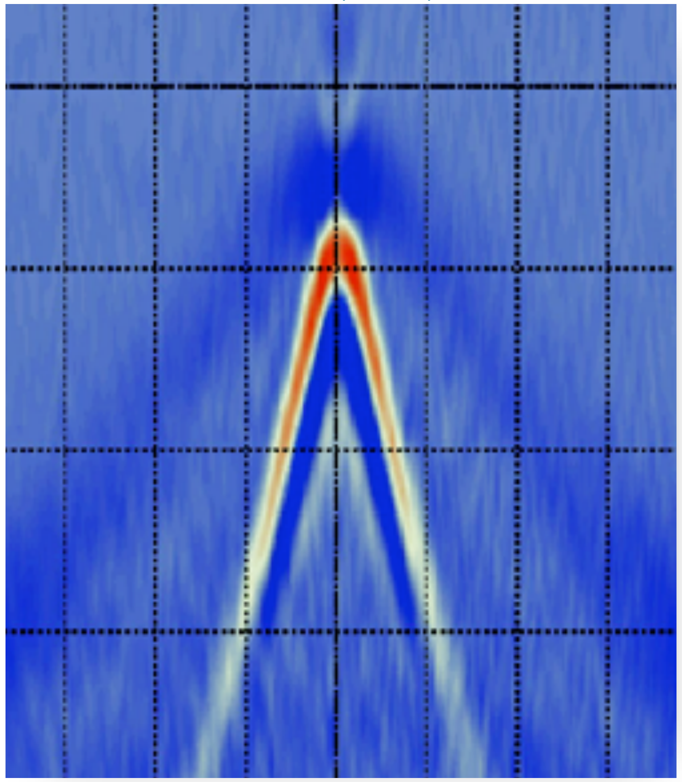
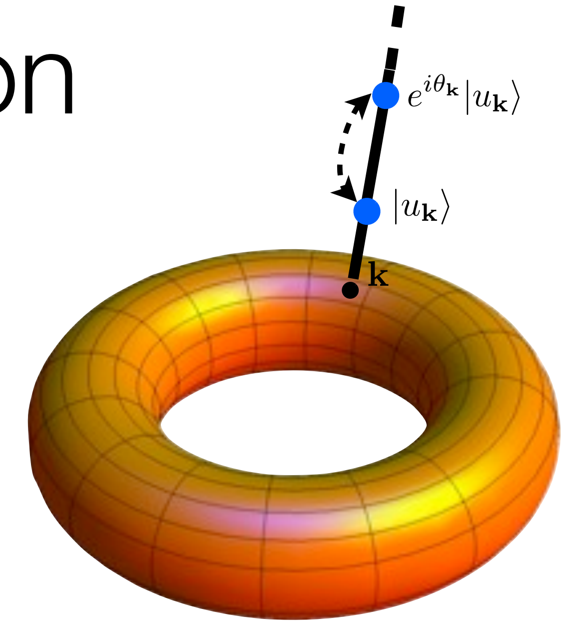


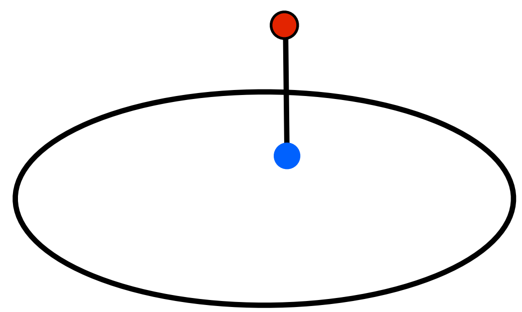
Main signature : robust Dirac surface states

Topology of bundles and Obstruction

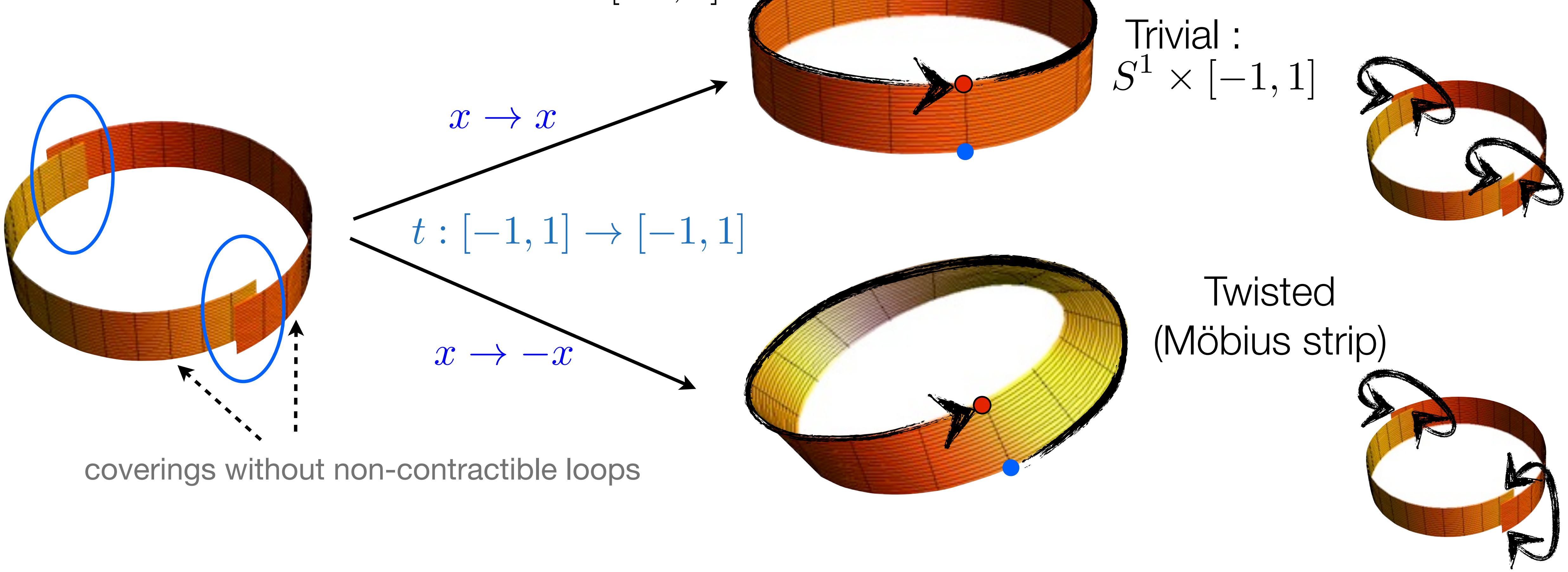


Twisted Valence Bloch Fiber bundles ?

Simpler Twisted Fiber bundles :

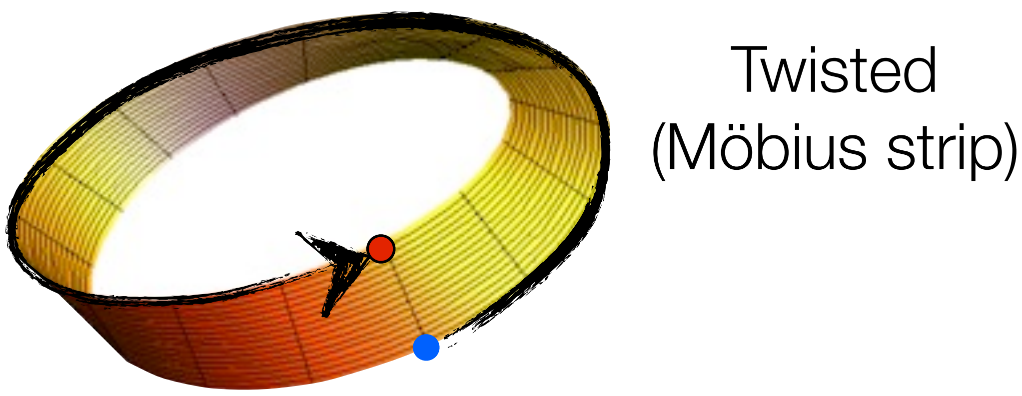


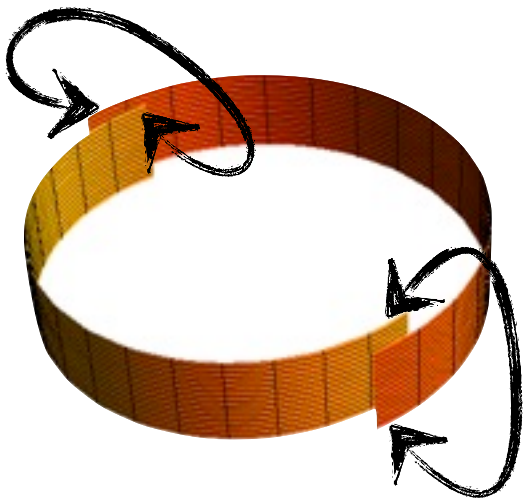
$S^1 \times [-1,1]$



Topology of bundles and Obstruction

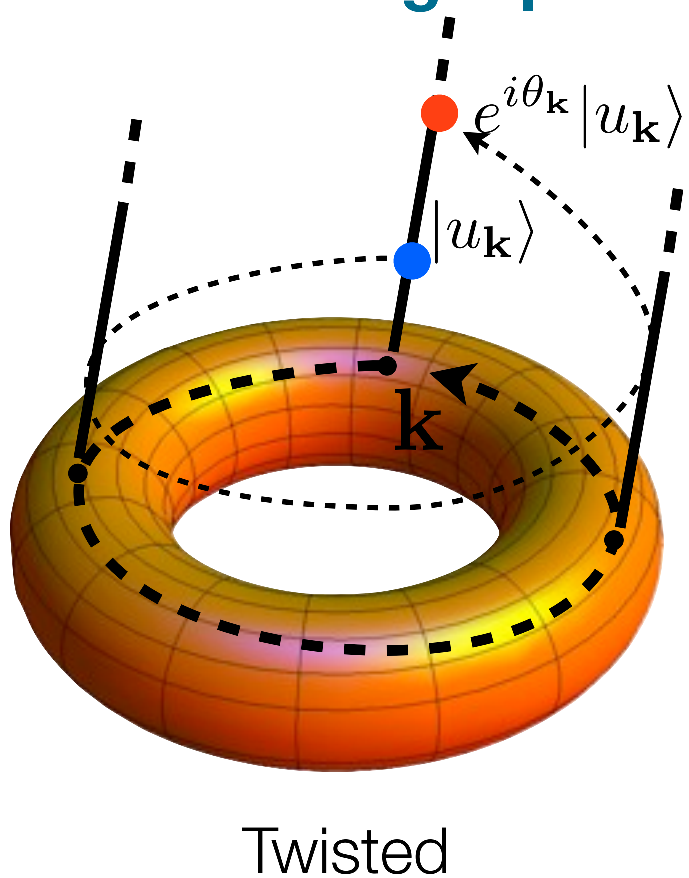
- Simple Fiber bundle $S^1 \times [-1,1]$

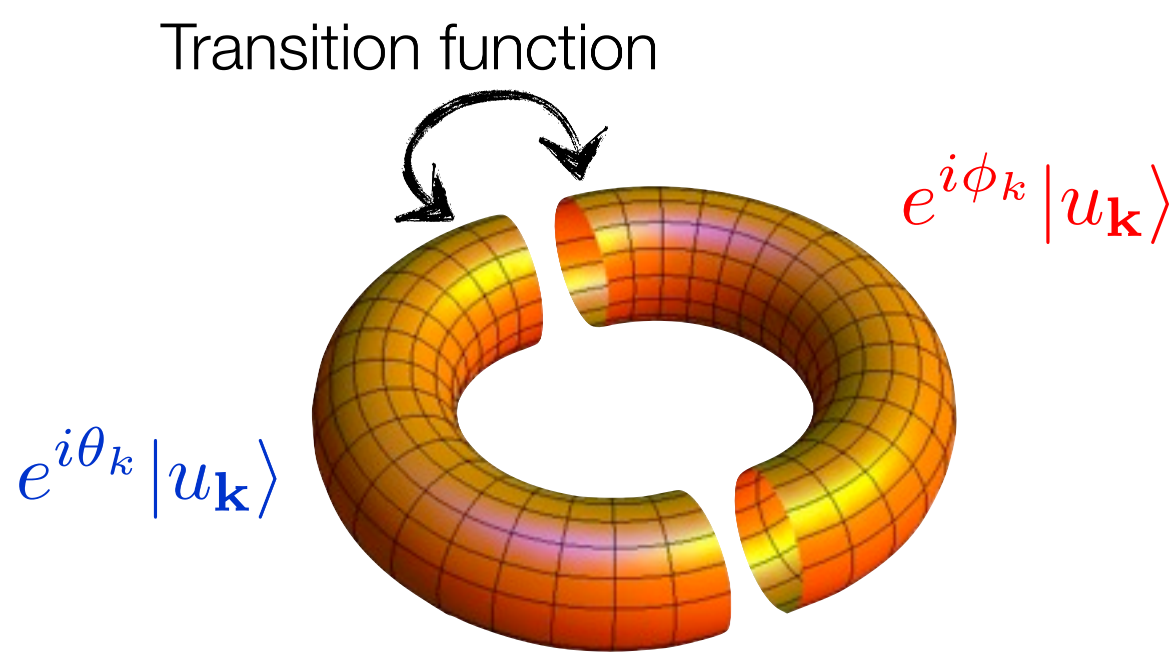




- Simple Bloch Bundle : Phase winding

$\Leftrightarrow$ **Obstruction to a single phase convention**





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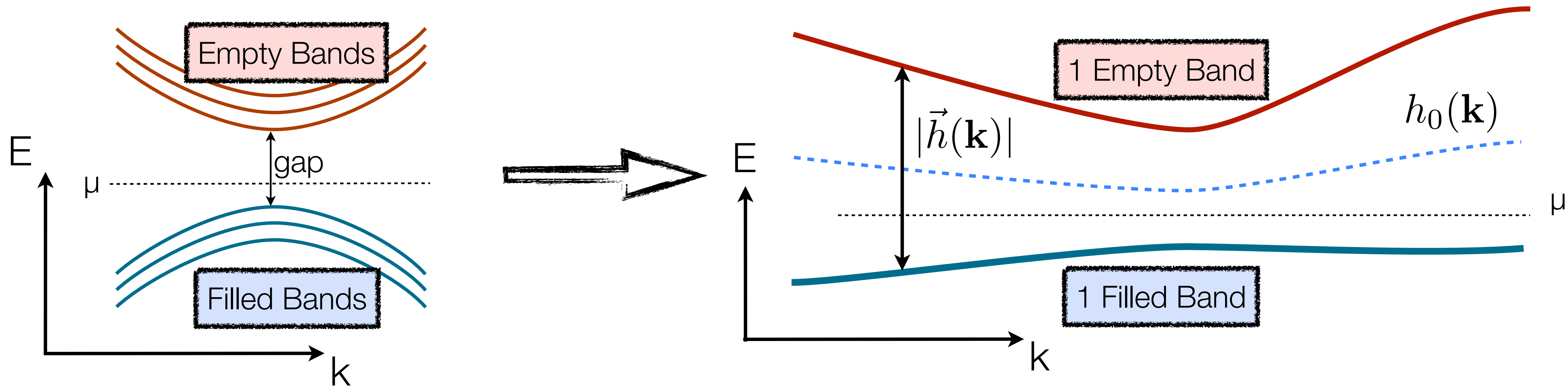
Topology and simple Two Bands Model

Thouless *et al.* (1982)
Haldane (1985)

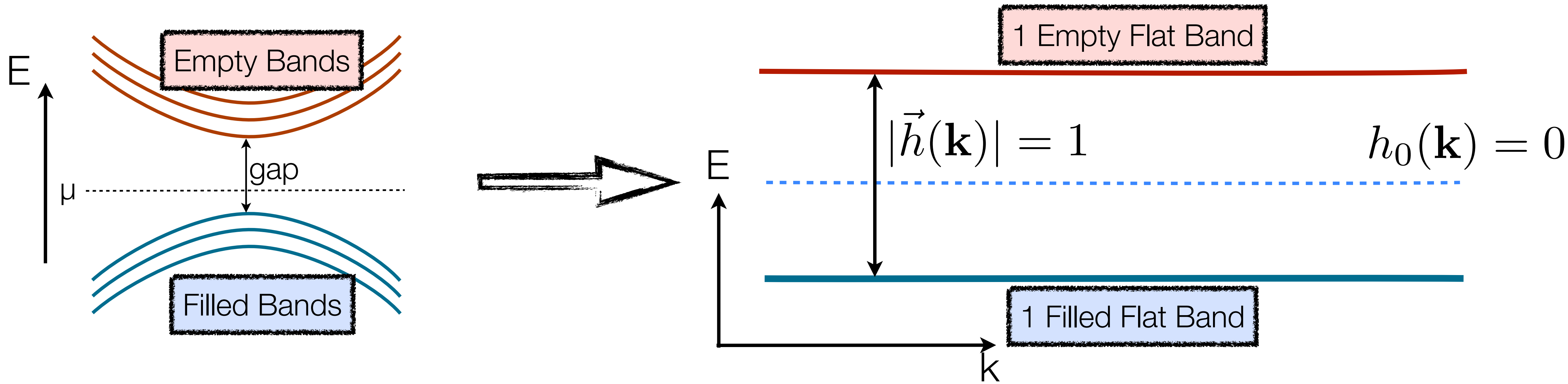


➡ Focus on (phase of) wave functions of the Filled Band of an Insulator

General Bloch Hamiltonian (Two Level System) :

$$H(\mathbf{k}) = \begin{pmatrix} h_0 + h_z & h_x - ih_y \\ h_x + ih_y & h_0 - h_z \end{pmatrix} = h_0(\mathbf{k})\mathbb{I} + \vec{h}(\mathbf{k}).\vec{\sigma}$$

Topology and simple Two Bands Model



➡ Focus on (phase of) wave functions of the Filled Band of an Insulator

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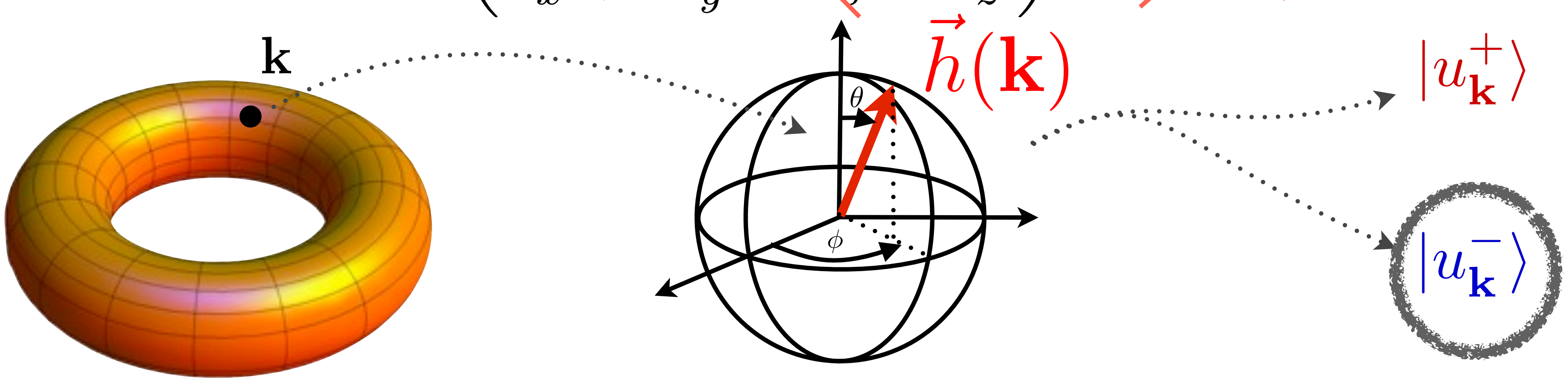

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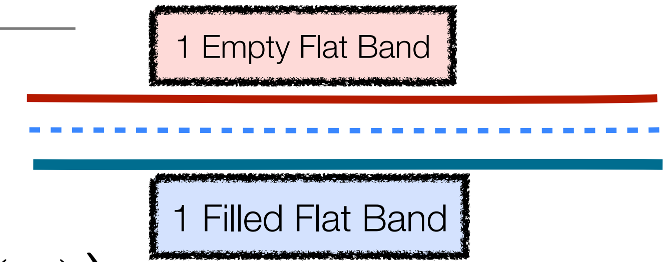
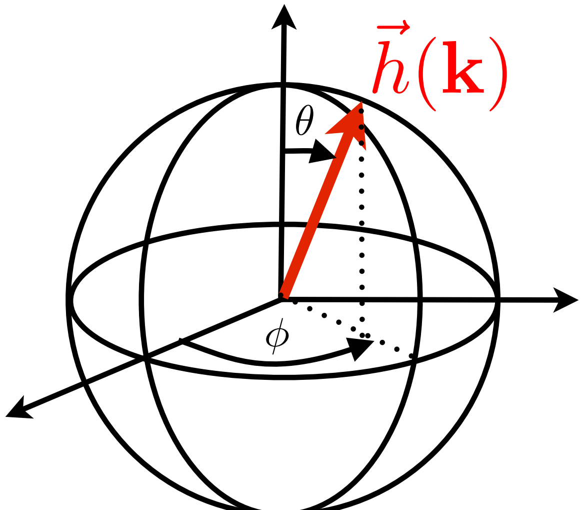
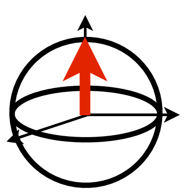


General Bloch Hamiltonian : $H(\mathbf{k}) = \vec{h}(\mathbf{k}).\vec{\sigma}$

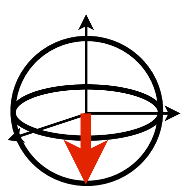


$$h(\mathbf{k}) = \begin{pmatrix} \sin\theta(\mathbf{k})\cos\phi(\mathbf{k}) \\ \sin\theta(\mathbf{k})\sin\phi(\mathbf{k}) \\ \cos\theta(\mathbf{k}) \end{pmatrix}$$

Eigenstates of the filled band : $|u_{\mathbf{k}}^-\rangle = \begin{pmatrix} \sin\frac{\theta(\mathbf{k})}{2} e^{-i\phi(\mathbf{k})} \\ -\cos\frac{\theta(\mathbf{k})}{2} \end{pmatrix}$

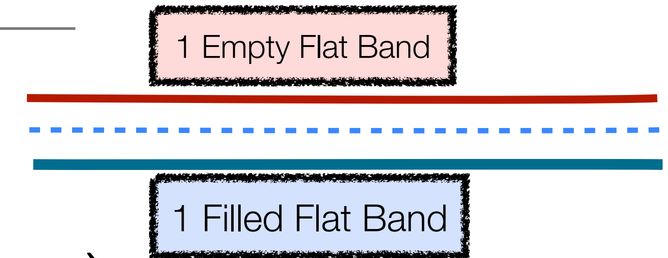


At the N pole : $|u^-\rangle = \begin{pmatrix} 0 \\ -1 \end{pmatrix}$



At the S pole : $|u^-\rangle = \begin{pmatrix} e^{-i\phi(\mathbf{k})} \\ 0 \end{pmatrix}$ not defined !

Topology and simple Two Bands Model



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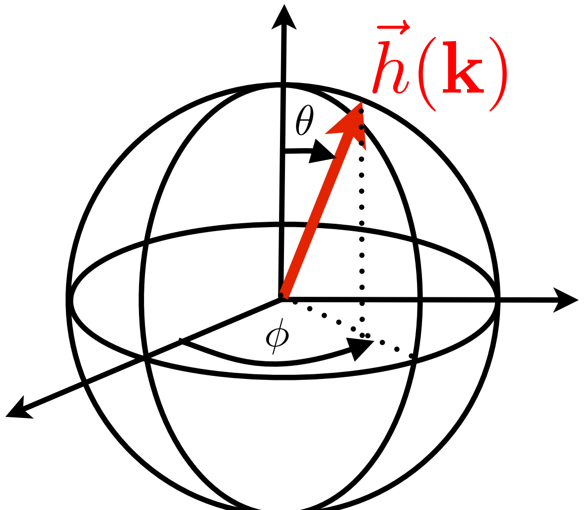

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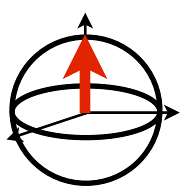
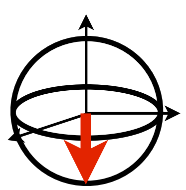
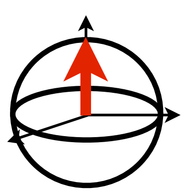


At the N pole : $|u^{-}\rangle = \begin{pmatrix} 0 \\ -1 \end{pmatrix}$

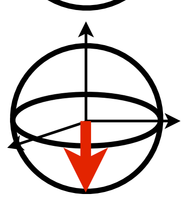


At the S pole : $|u^{-}\rangle = \begin{pmatrix} e^{-i\phi(\mathbf{k})} \\ 0 \end{pmatrix}$ not defined !

Alternative choice of phase : $|\tilde{u}_{\mathbf{k}}^{-}\rangle = e^{i\phi(\mathbf{k})}|u_{\mathbf{k}}^{-}\rangle = \begin{pmatrix} \sin\frac{\theta(\mathbf{k})}{2} \\ -\cos\frac{\theta(\mathbf{k})}{2} e^{i\phi(\mathbf{k})} \end{pmatrix}$

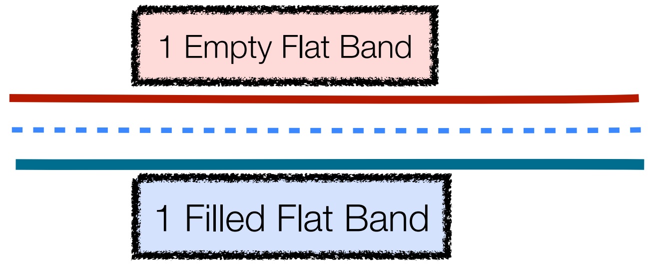


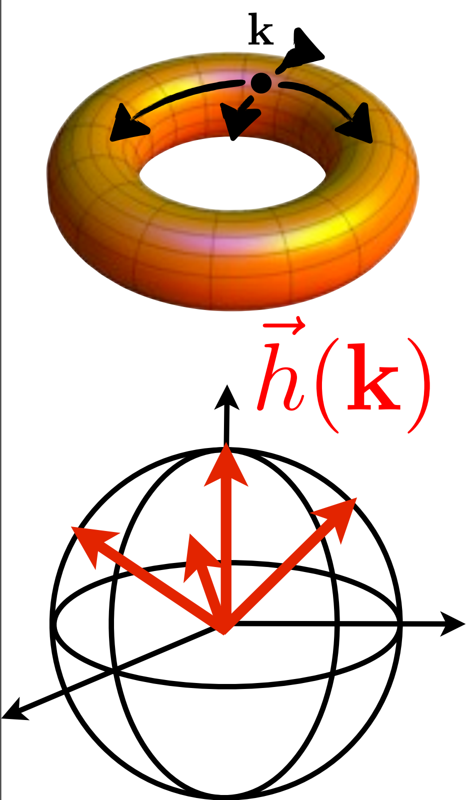
At the N pole : $|\tilde{u}^{-}\rangle = \begin{pmatrix} 0 \\ -e^{i\phi(\mathbf{k})} \end{pmatrix}$ not defined !



At the S pole : $|\tilde{u}^{-}\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$

Topology and Two Bands Model

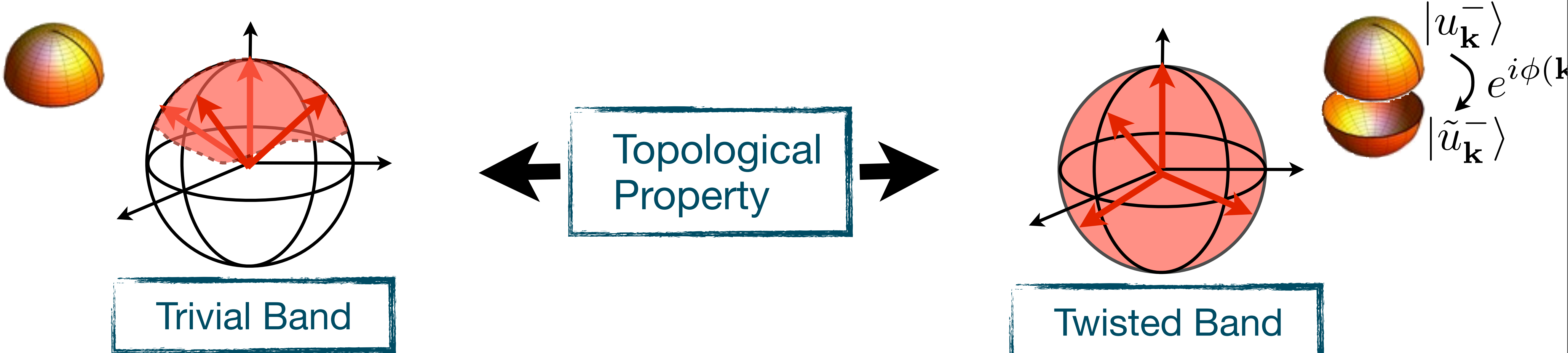




It is not possible to have a coherent phase convention for all points $\vec{h}$ of the sphere

- if $\vec{h}(\mathbf{k})$ does not cover the whole sphere : single phase convention possible. «Standard trivial case»
- If $\vec{h}(\mathbf{k})$ spreads over the whole sphere : we need 2 independent phase conventions

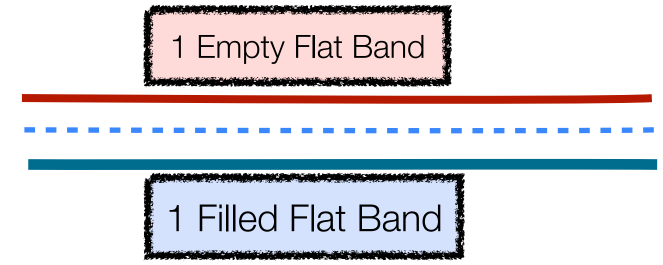
➡ signals a topological property : the wavefunction phase winds by 2π around the sphere



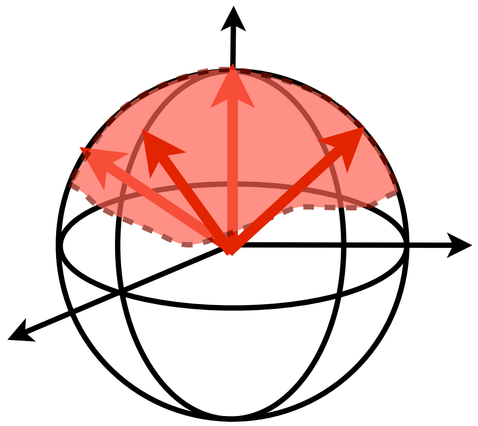
single phase convention possible

Chern number $\Longleftrightarrow$ winding of electronic phase

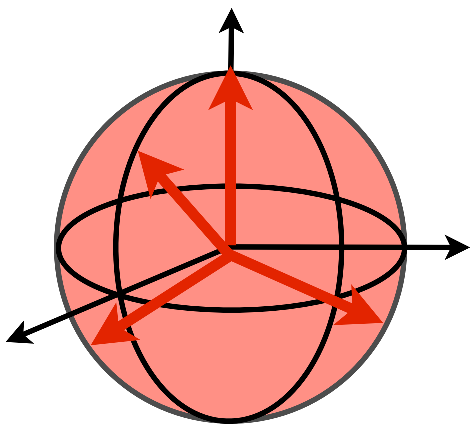
Topology and Two Bands Model



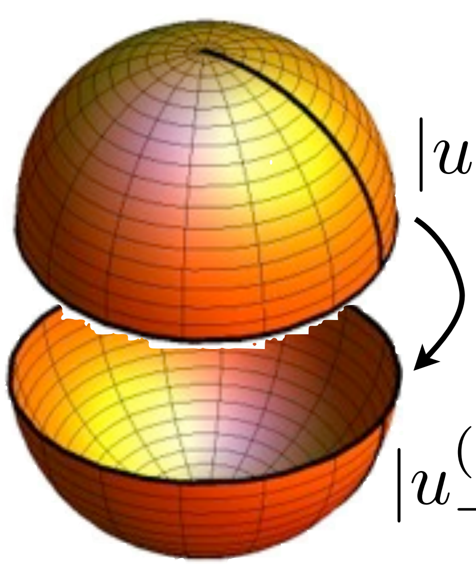
Topological Index to detect non-triviality : Chern number



- physicist like the Berry connection : $A = \frac{1}{i}\langle u_- | \mathrm{d}\, u_- \rangle$
- Berry curvature $F = \mathrm{d}A$
- (first) Chern number : $C_1 = \frac{1}{2\pi}\int_{\mathrm{BZ}} F$



- measures the 'triviality' of the transition function :



$|u_-^{(N)}(\mathbf{k})\rangle$

$t^{(NS)}(\mathbf{k}) = e^{i\phi(\mathbf{k})}$

$|u_-^{(S)}(\mathbf{k})\rangle$

$$\begin{aligned} C_1 &= \frac{1}{2\pi}\int_{\mathrm{BZ}} F \\ &= \frac{1}{2\pi}\left[\int_{h^{-1}(U_N)} F + \int_{h^{-1}(U_S)} F\right] \\ &= \frac{1}{2\pi}\left[\int_{\partial h^{-1}(U_N)} h^\star A_N + \int_{\partial h^{-1}(U_S)} h^\star A_S\right] \end{aligned}$$

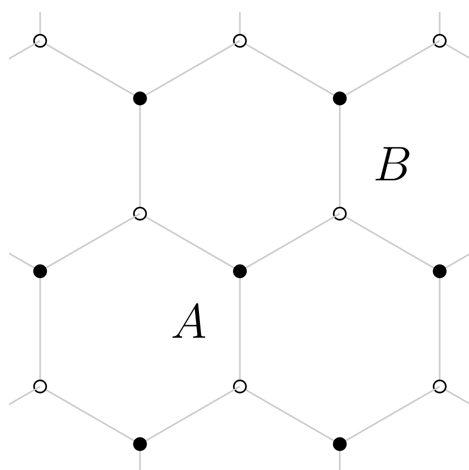
and $A_N - A_S = d\varphi = \frac{1}{i} d\log(t_{NS})$

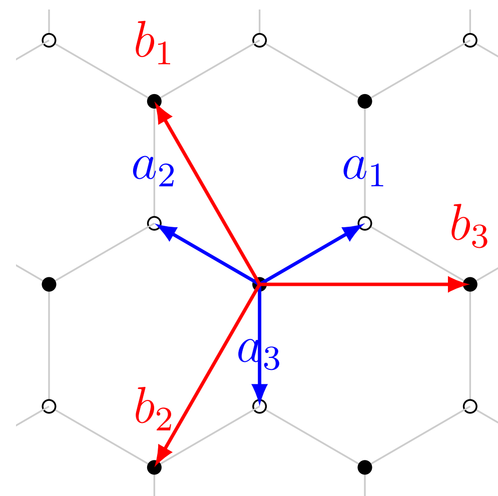
$$\Rightarrow C_1 = 1$$

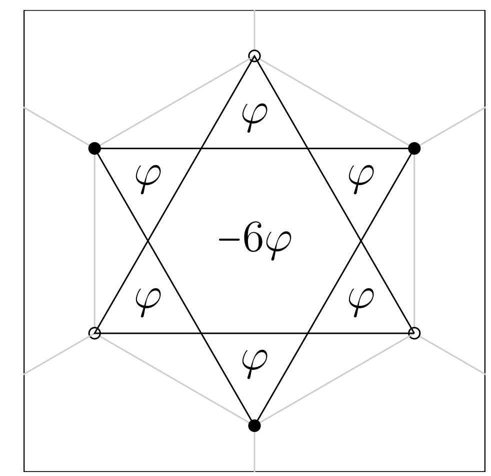
Chern Topological Order : explicit model

Haldane (1985)

2 sublattices : A and B







staggered fluxes inside unit cell

$$H = t \sum_{\langle i,j \rangle} |i\rangle\langle j| + t_2 \sum_{\langle\langle i,j \rangle\rangle} |i\rangle\langle j| + M \left[\sum_{i \in A} |i\rangle\langle i| - \sum_{i \in B} |i\rangle\langle j| \right]$$

In the (A,B) basis :

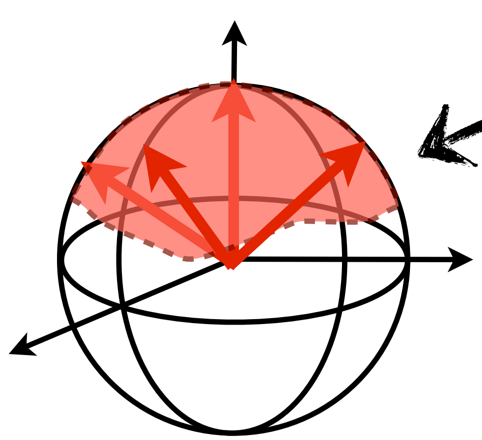
$$H(\mathbf{k}) = \begin{pmatrix} h_0 + h_z & h_x - ih_y \\ h_x + ih_y & h_0 - h_z \end{pmatrix} = h_0(\mathbf{k})\mathbb{I} + \vec{h}(\mathbf{k}).\vec{\sigma}$$

$$h_0 = 2t_2 \cos\phi \sum_{i=1}^{3} \cos(k \cdot b_i)$$

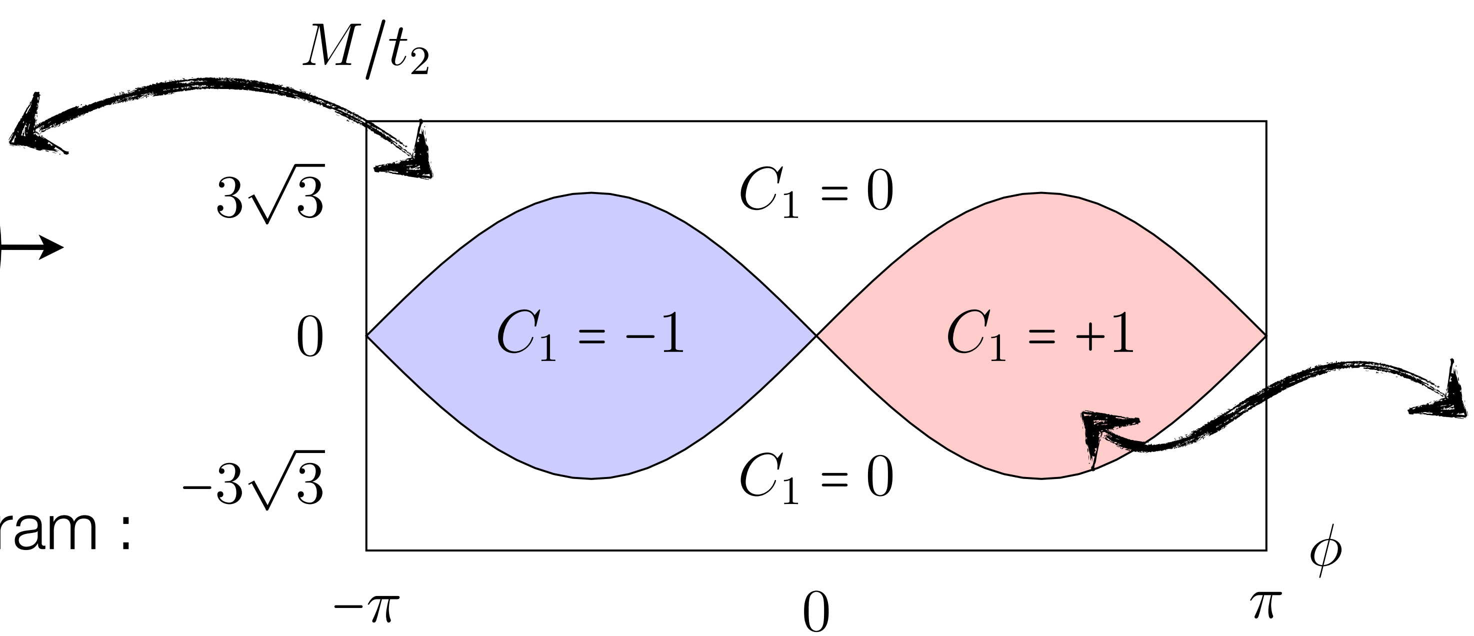
$$h_x = t\,(1 + \cos(k \cdot b_1) + \cos(k \cdot b_2))$$

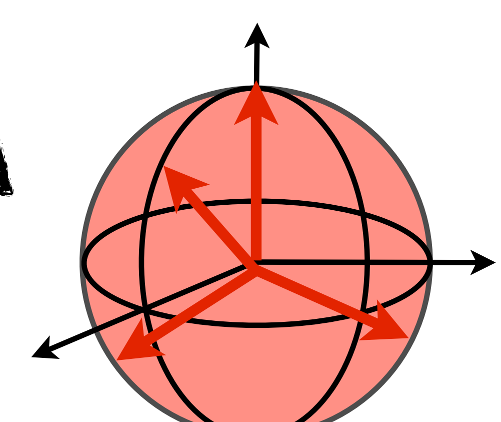
$$h_y = t\,(1 + \sin(k \cdot b_1) - \sin(k \cdot b_2))$$

$$h_z = M - 2t_2 \sin\phi \sum_{i=1}^{3} \cos(k \cdot b_i)$$



Phase Diagram :





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Purpose : illustrate topological orders as an obstruction using simple models

Time Reversal Symmetry

Property of Time Reversal in Quantum Mechanics (for spin ½) :

- action **T** : **k** →-**k** ; σ →-σ $\left(T = e^{\frac{i}{\hbar}\pi S_y}\ K\ \right)$
- **T^2=-I** (rotation by 2π of spin ½)
- Kramers degeneracy : if |u⟩ is an eigenstate of H, then T|u⟩ is a distinct eigenstate with same energy

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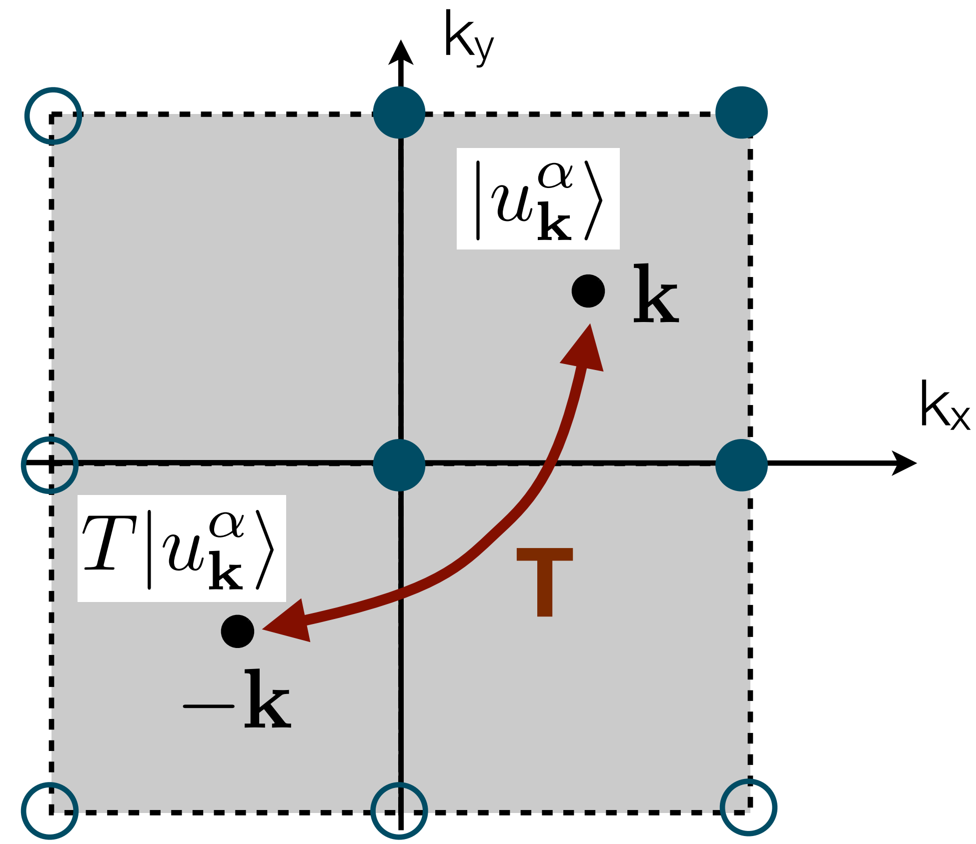
Application to bands in a crystal :
Time reversal symmetry

- Relates spectrum at **k** and -**k**



Brillouin Zone

Time Reversal Symmetry

Property of Time Reversal in Quantum Mechanics (for spin ½) :

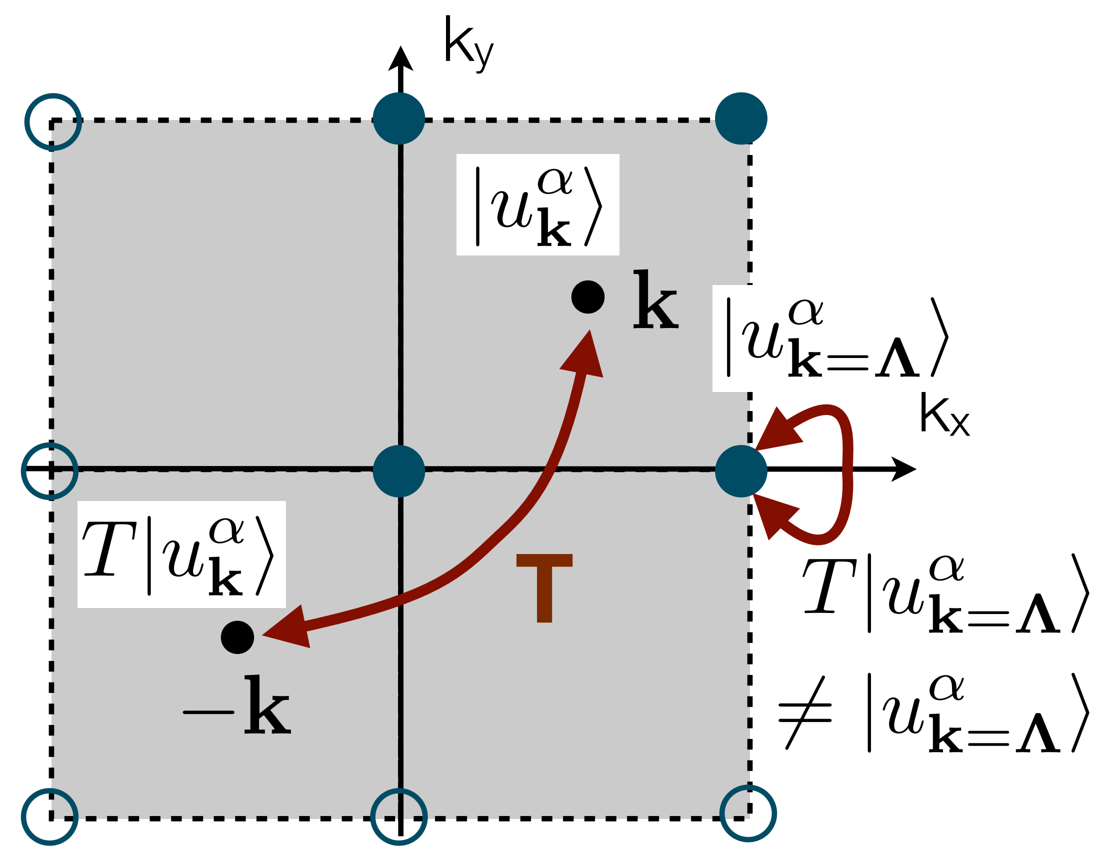
- action **T** : **k** →-**k** ; σ →-σ $(T = e^{\frac{i}{\hbar}\pi S_y} K)$
- **T²=-I** (rotation by 2π of spin ½)
- Kramers degeneracy : if |u〉 is an eigenstate of H, then T|u〉 is a distinct eigenstate with same energy

Application to bands in a crystal :
Time reversal symmetry

- Relates spectrum at **k** and -**k**
- Except at the Time Reversal Invariant Momenta Λ_i(●) where

-**k** = **k** +**G**

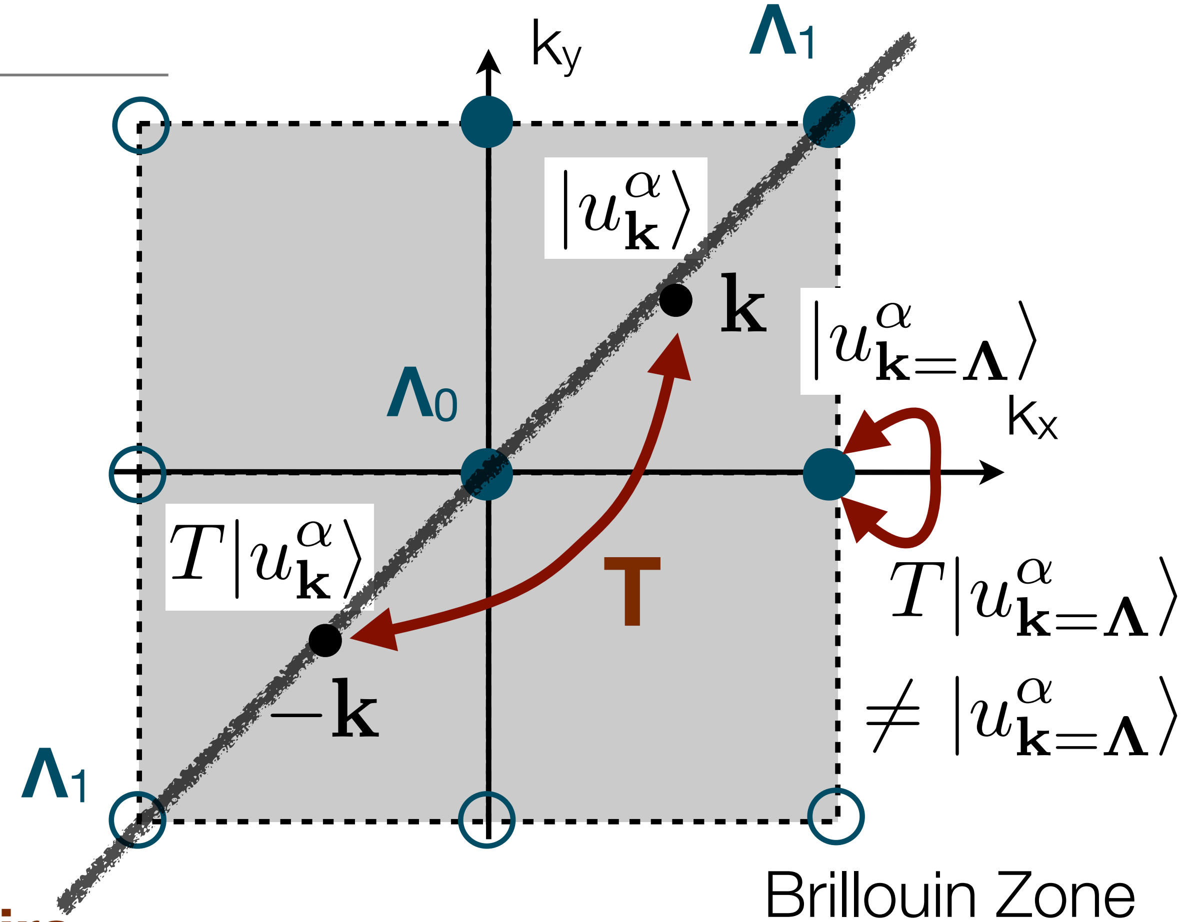
⇒ imposes degeneracy

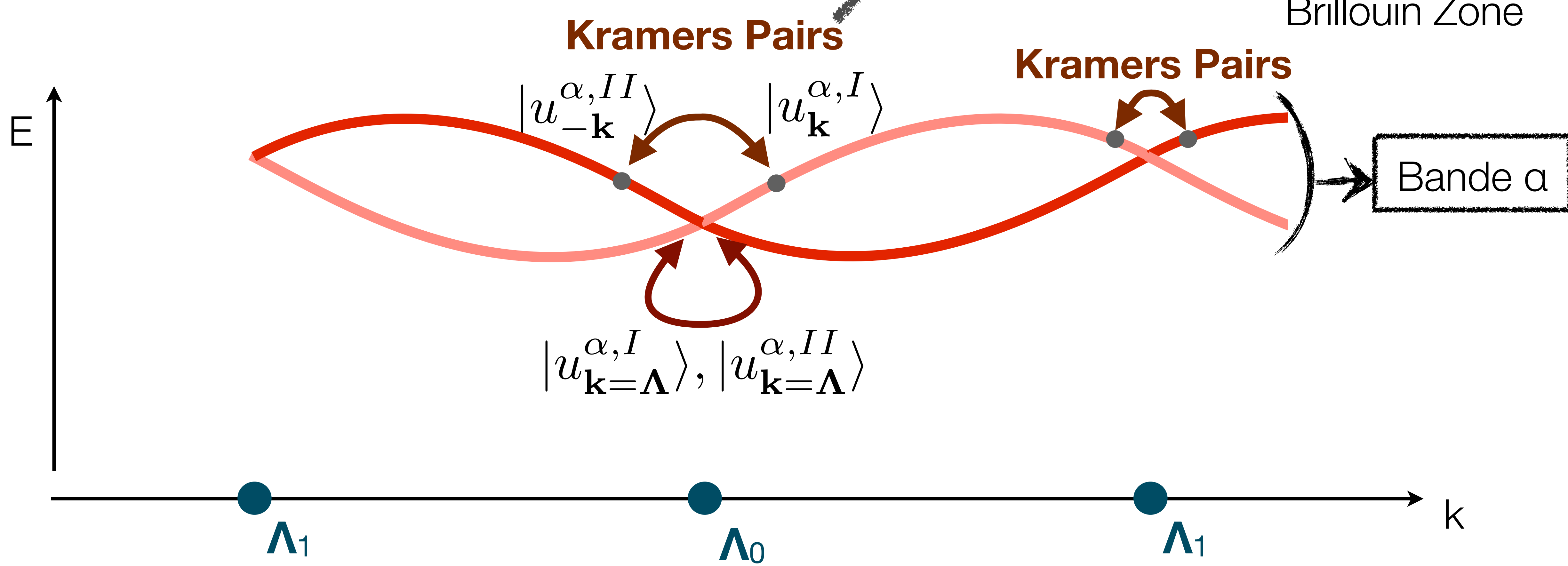


Brillouin Zone

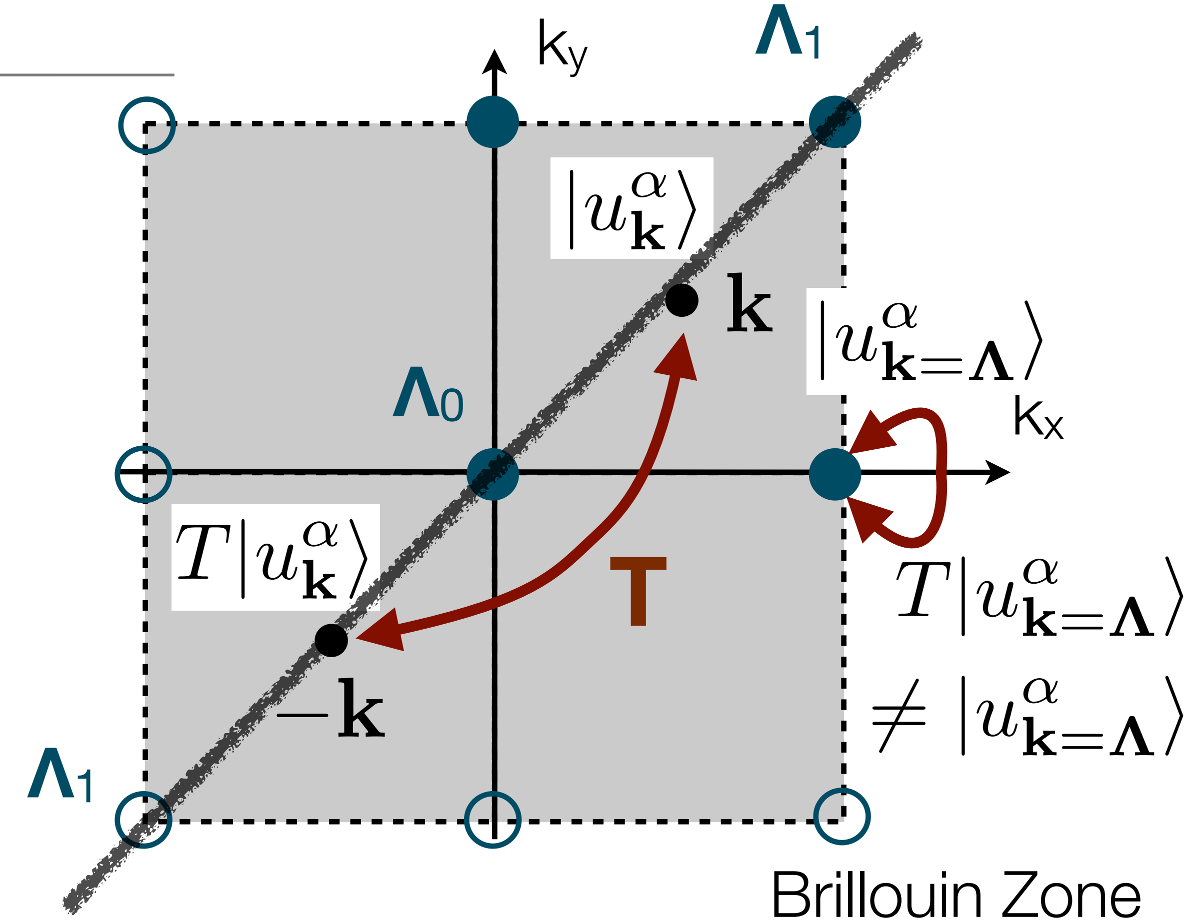
Time Reversal Symmetry

➡ Typical energy spectrum with T symmetry

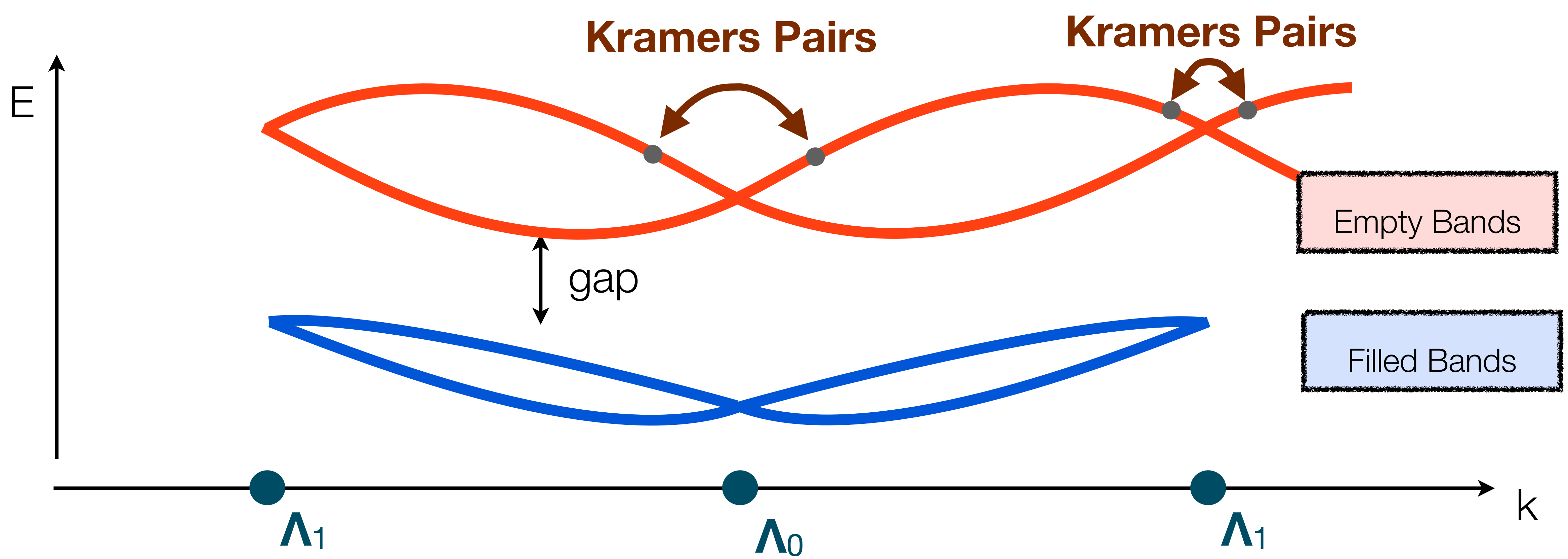




Time Reversal Symmetry



Insulator structure : minimum **4 bands**



Inversion / Parity Symmetry

- Time Reversal Symmetry : relates state $|u^{\alpha,I}_{\mathbf{k}}\rangle$ and $|u^{\alpha,II}_{-\mathbf{k}}\rangle$
  (exchanges spin quantum numbers)
- Inversion/Parity Symmetry x→-x relates state $|u^{\alpha,I}_{\mathbf{k}}\rangle$ and $|u^{\alpha,I}_{-\mathbf{k}}\rangle$
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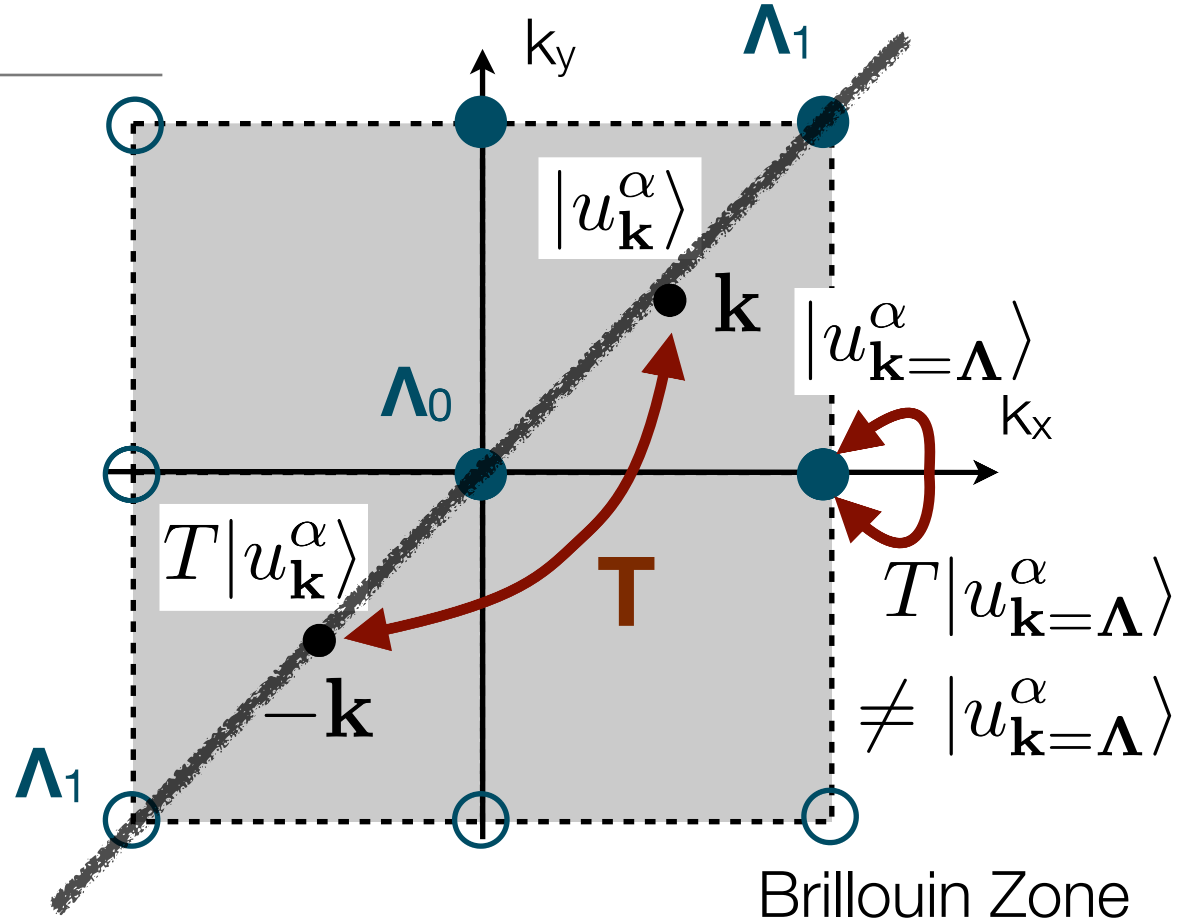
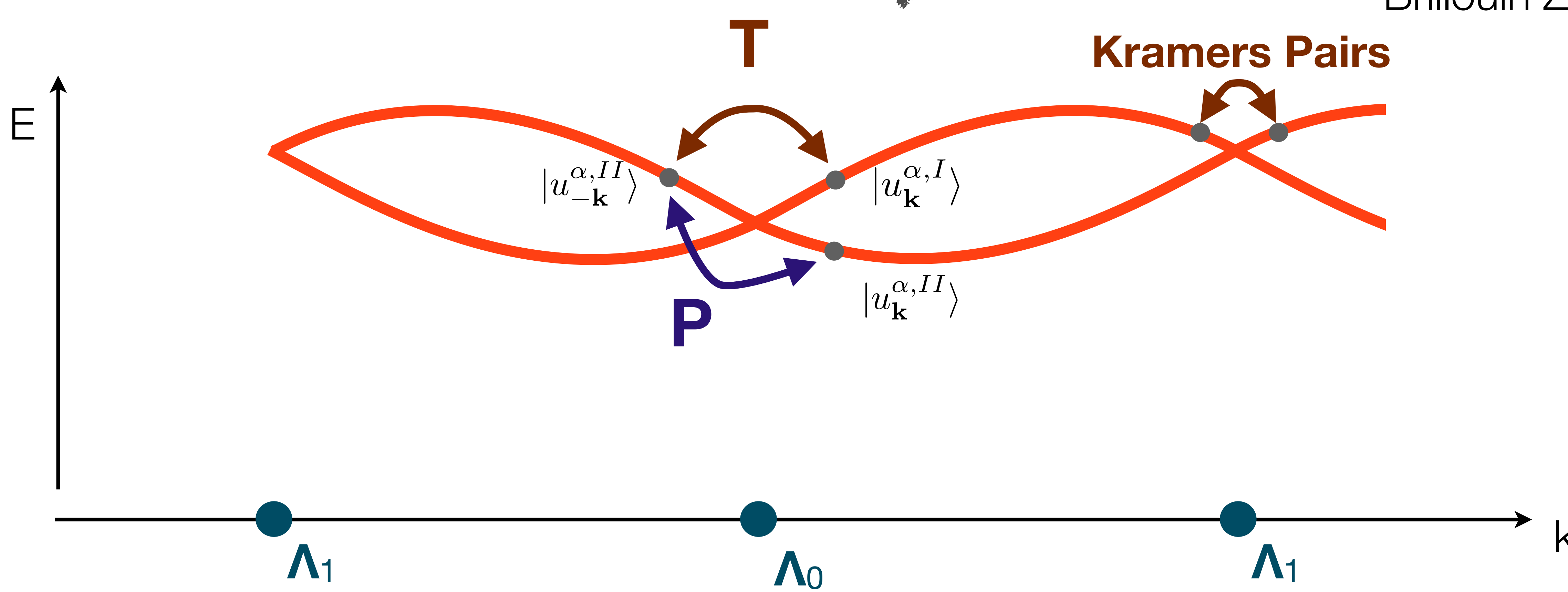


If P and T are symmetries ...



Inversion / Parity Symmetry

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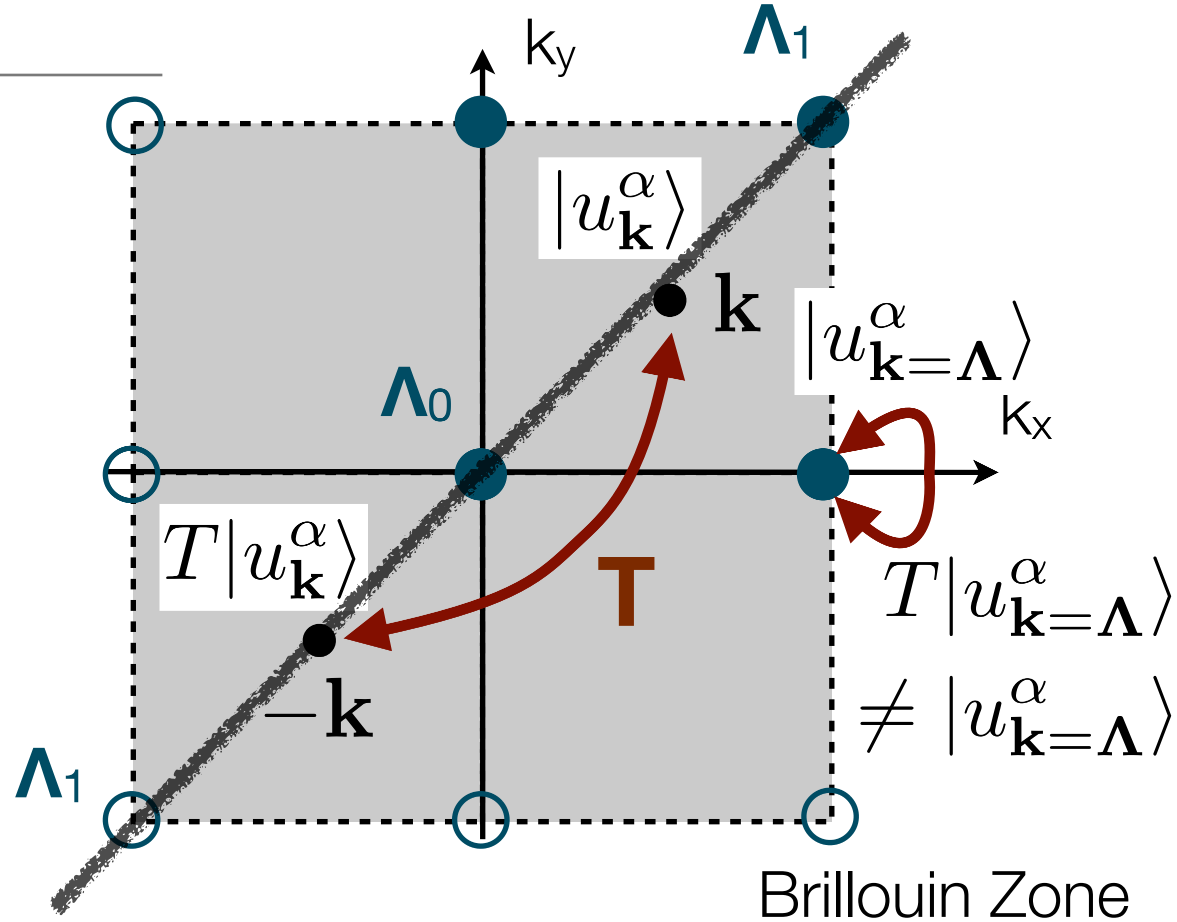
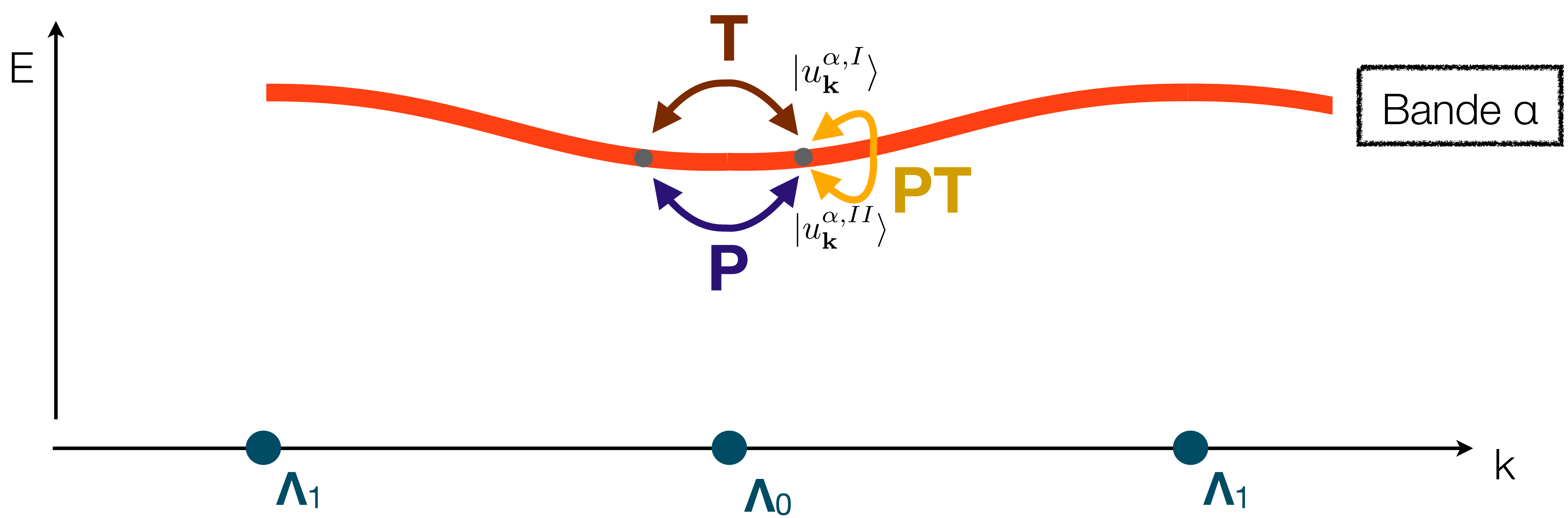


If P and T are symmetries ...

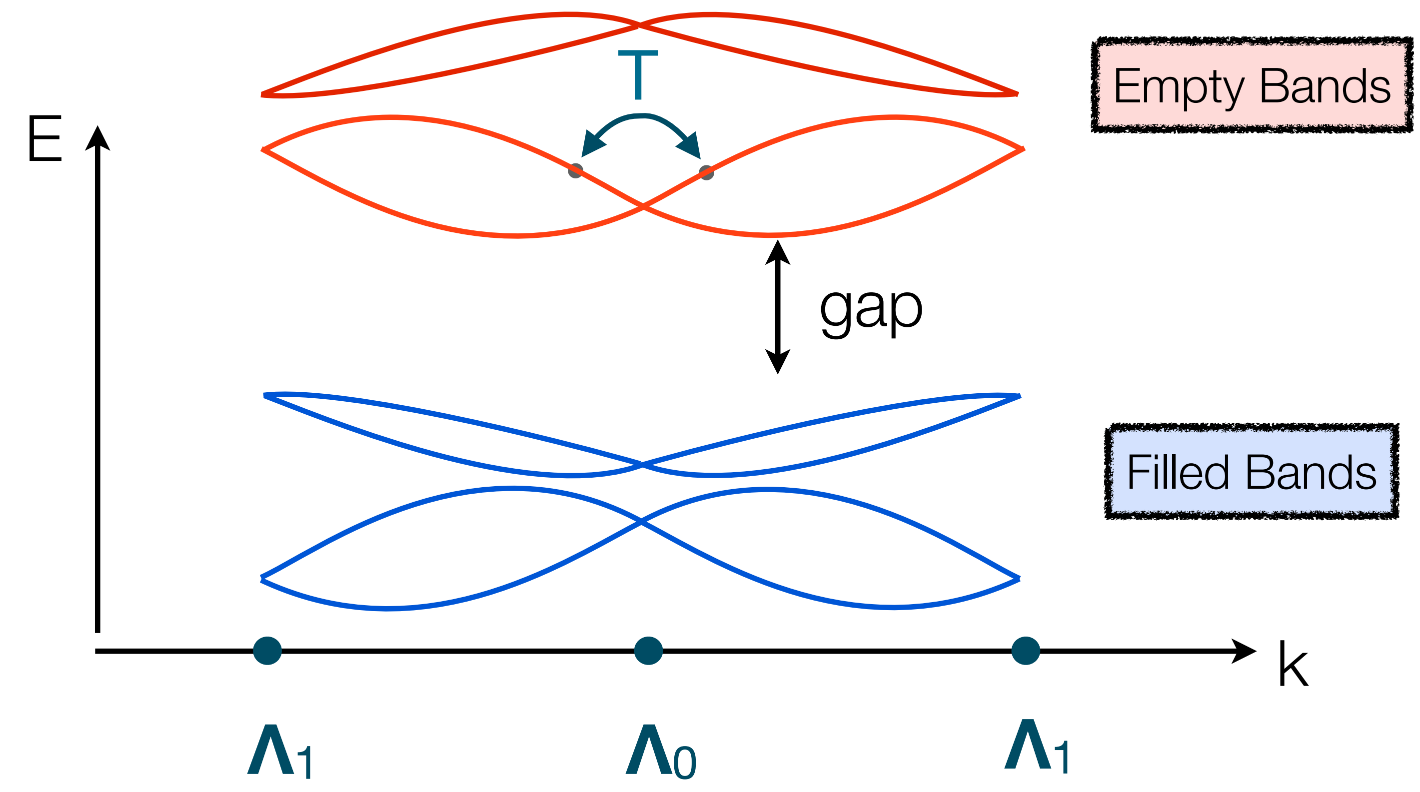
... the bands are degenerate



Z_2 Topological Order in a simplified Four Bands Model

C.L.Kane and E.J.Mele PRL **95** (2005)
Fu, Kane, PRB **76** (2007)
Bernevig, Hughes and Zhang, Science **314** (2006)

- Spin dependent Time Reversal Symmetric Insulator band structure



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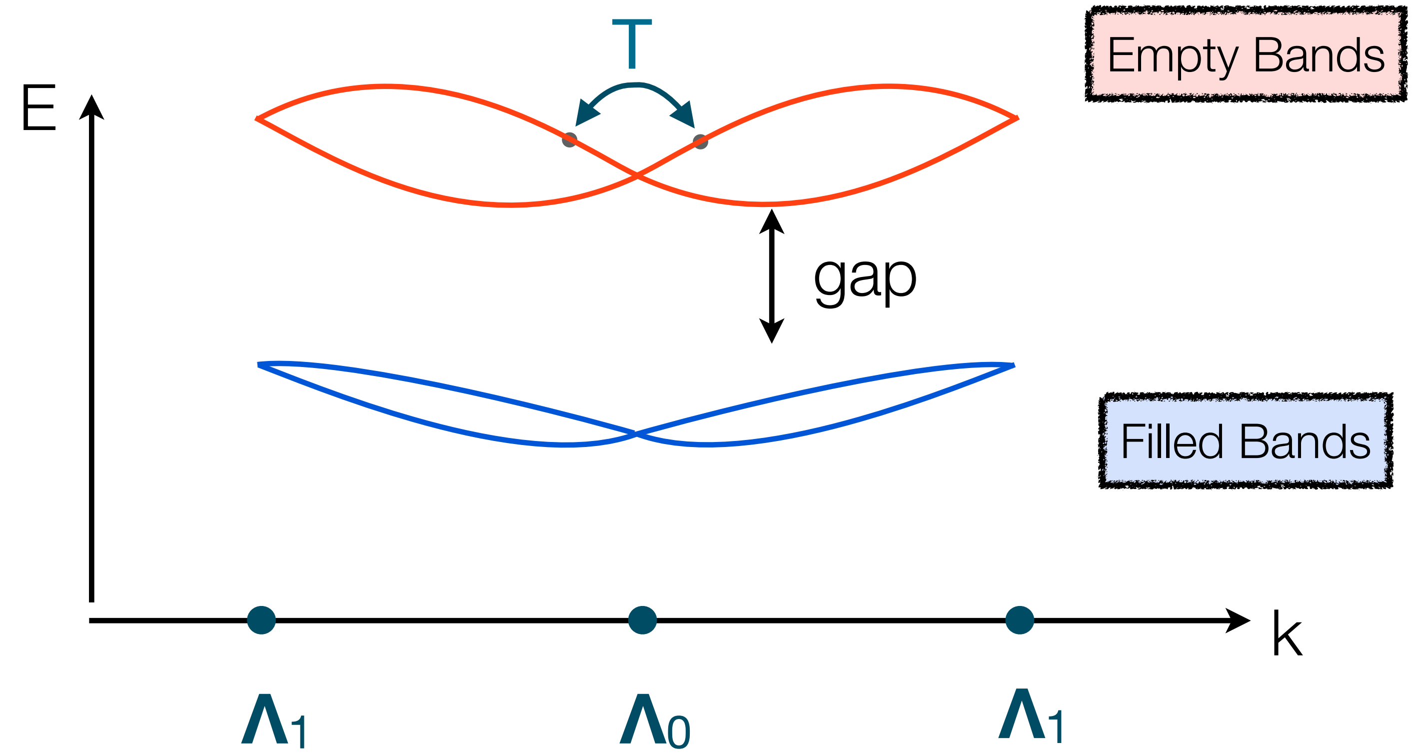
- Spin dependent Time Reversal Symmetric Insulator band structure
- Simplest Spin dependent Hamiltonian Time Reversal Symmetric :

  Four Level System, two spin ½ : σ⊗S



Bloch Hamiltonian parametrized as

$$H(k) = d_0(\mathbf{k})\mathbb{I} + \sum_{i=1}^{5} d_i(\mathbf{k})\,\Gamma_i \; + \sum_{i>j} d_{ij}(\mathbf{k})\,\Gamma_{ij}$$

- 5 Dirac matrices : $\{\Gamma_a, \Gamma_b\} = 2\delta_{a,b}$
- 10 additional matrices : $\Gamma_{a,b} = \frac{1}{2i}\,[\Gamma_a, \Gamma_b]$

vendredi 13 septembre 13

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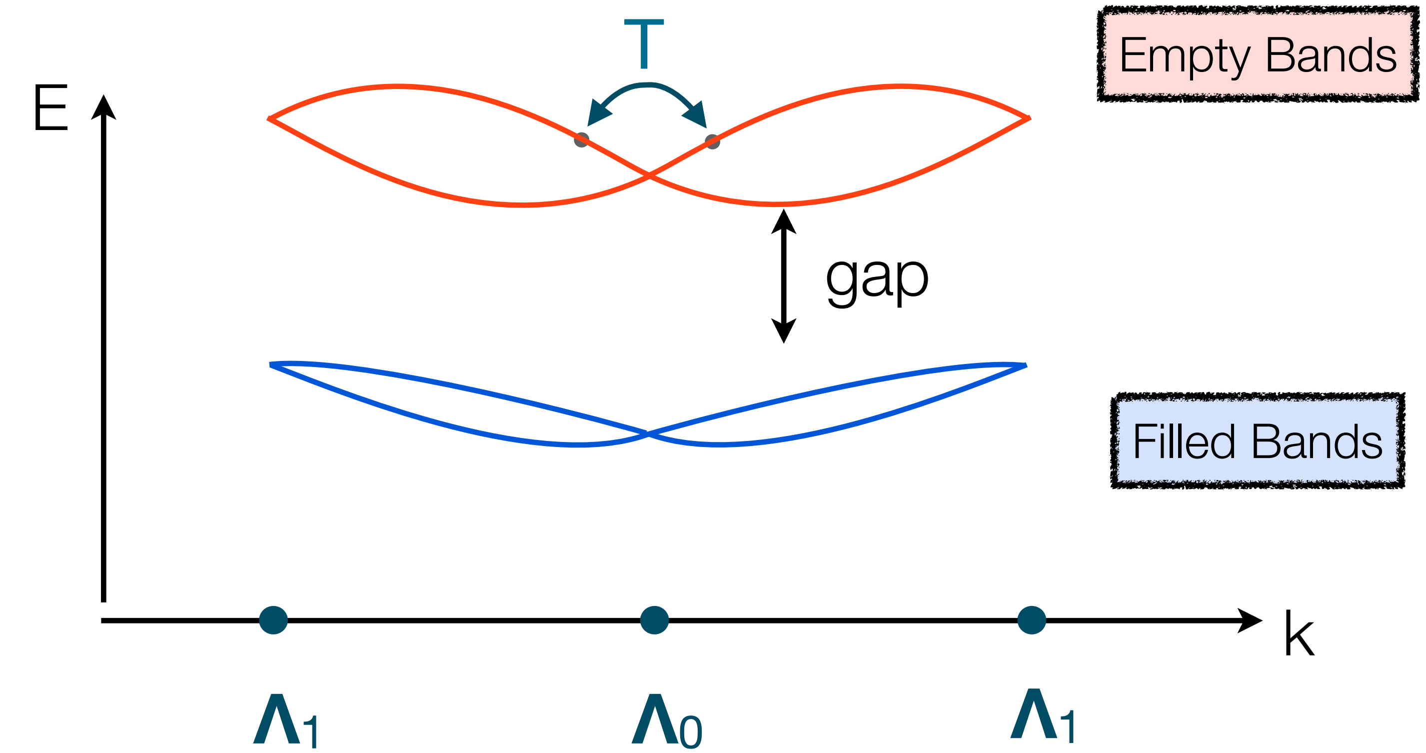

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We can choose :

- Γ_1 as the Parity operator P : **k→-k**
- matrices $\Gamma_{i>1}$ are even under PT : $(PT)\Gamma_i(PT)^{-1} = \Gamma_i$
- matrices Γ_{ij} are odd under PT : $(PT)\Gamma_{ij}(PT)^{-1} = -\Gamma_{ij}$

... Simplest model : keep only 3 matrices

Two Historical Simple models

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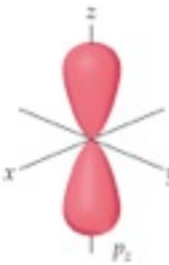
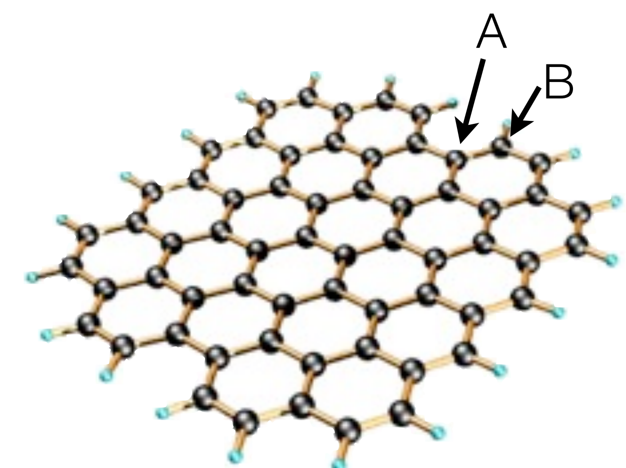
$$H(k) = d_1(k)\,\Gamma_1 \ + \ d_2(k)\,\Gamma_2 + d_3(k)\,\Gamma_3$$

1. Kane Mele Model

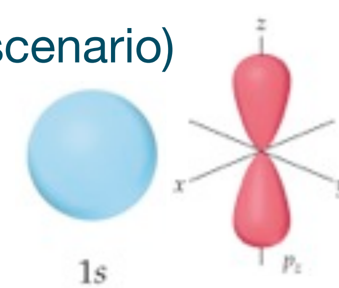


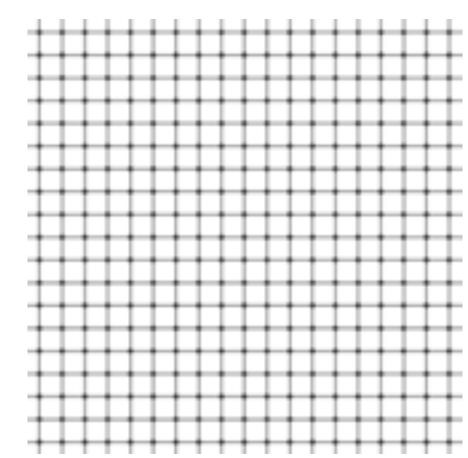


- Identical atomic orbitals (e.g. p_z)
- bipartite lattice (graphene) with 2 sublattices A and B
- Sublattice basis : $(A\uparrow, A\downarrow, B\uparrow, B\downarrow)$
- Parity operator : exchanges A and B sublattices : $\Gamma_1 = \sigma_x \otimes I$
- $\Gamma_2 = \sigma_y \otimes I$, $\Gamma_3 = \sigma_z \otimes s_z$

2. Bernevig-Hughes-Zhang Model

(band inversion scenario)





- Atomic orbitals with opposite parity (e.g. s,p_z)
- Parity basis : $(s\uparrow, s\downarrow, p\uparrow, p\downarrow)$
- Parity operator : diagonal, : $\Gamma_1 = \sigma_z \otimes I$
- $\Gamma_2 = \sigma_y \otimes I$, $\Gamma_3 = \sigma_x \otimes s_z$

... different band structures, but same Z_2 topological order

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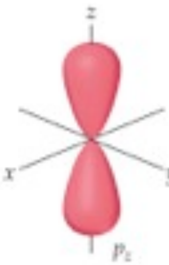

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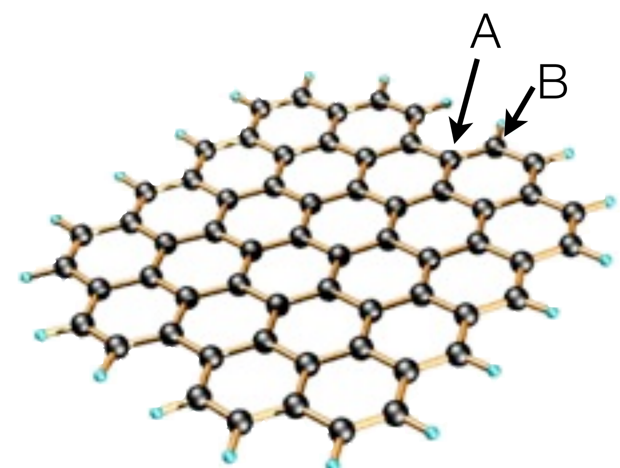

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Kane-Mele model

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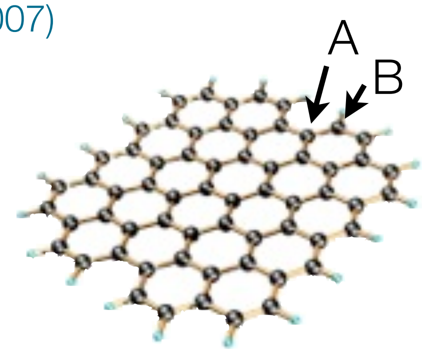


Four Level System, two spin ½ (σ ⊗ S) : $(A\uparrow, A\downarrow, B\uparrow, B\downarrow)$

$$H(k) = d_1(k)\,\Gamma_1 + d_2(k)\,\Gamma_2 + d_3(k)\,\Gamma_3$$

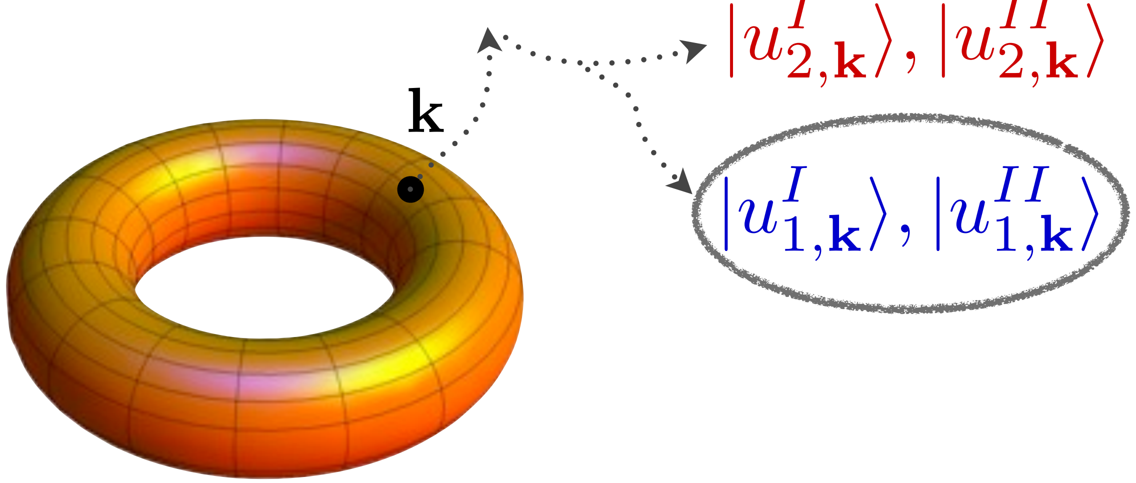
- Parity operator (A↔B) : $\Gamma_1 = \sigma_x \otimes I$
- $\Gamma_2 = \sigma_y \otimes I$, $\Gamma_3 = \sigma_z \otimes s_z$
- Time Reversal Operator : $T = i\,(I \otimes s_y).K$

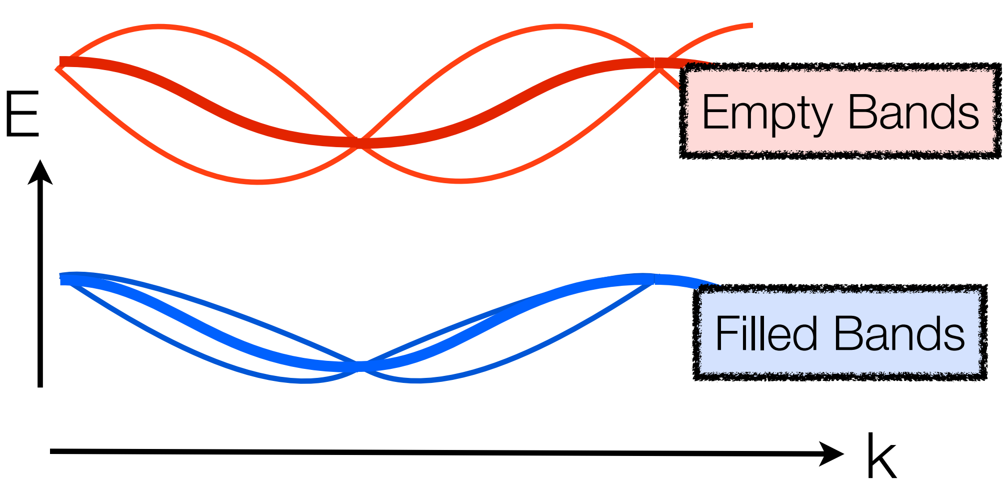
Complex Conjugation

Purpose :

- impose insulator band structure (gap)
- determine the eigenfunctions of the filled bands (obstruction or not ?)

$\{d_1(k), d_2(k), d_3(k)\}$





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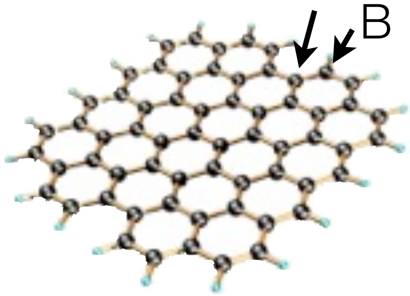

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$\Gamma_1 = \sigma_x \otimes I$, $\Gamma_2 = \sigma_y \otimes I$, $\Gamma_3 = \sigma_z \otimes s_z$

- Eigenenergies : $E_{1/2}(\mathbf{k}) = \pm\sqrt{d_1^2(\mathbf{k}) + d_2^2(\mathbf{k}) + d_3^2(\mathbf{k})}$

  ➡ $d_1(\mathbf{k}), d_2(\mathbf{k}), d_3(\mathbf{k})$ cannot simultaneously vanish

- Eigenstates of the filled band (arbitrary phase convention) :

$$|u^{I}_{1,\mathbf{k}}\rangle = \frac{1}{\mathcal{N}_1}\begin{pmatrix} 0 \\ -d_3 - ||d|| \\ 0 \\ d_1 + id_2 \end{pmatrix} \qquad |u^{II}_{1,\mathbf{k}}\rangle = \frac{1}{\mathcal{N}_1}\begin{pmatrix} d_3 - ||d|| \\ 0 \\ d_1 + id_2 \\ 0 \end{pmatrix}$$

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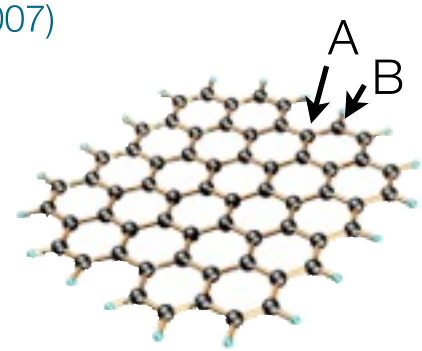

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states ill-defined for $d_1 + id_2 = te^{i\theta} \to 0$

$$|u^I_1\rangle \to \begin{pmatrix} 0 \\ -1 \\ 0 \\ 0 \end{pmatrix} \quad \text{and} \quad |u^{II}_1\rangle \to \begin{pmatrix} 0 \\ 0 \\ e^{i\theta} \\ 0 \end{pmatrix} \quad (d_3 > 0)$$

$$|u^I_1\rangle \to \begin{pmatrix} 0 \\ 0 \\ 0 \\ e^{i\theta} \end{pmatrix} \quad \text{and} \quad |u^{II}_1\rangle \to \begin{pmatrix} -1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \quad (d_3 < 0)$$

Does $d_1 = d_2 = 0$ occurs ?

Kane-Mele model

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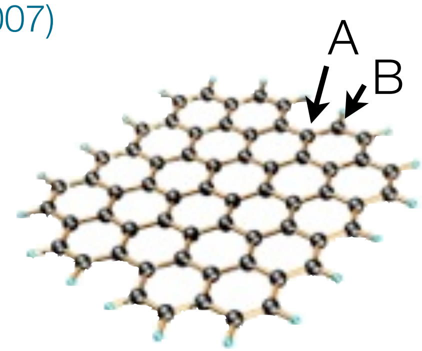

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Symmetry constraints :

$P = \Gamma_1$: $P\,\Gamma_1\,P^{-1} = \Gamma_1$, $T\,\Gamma_1\,T^{-1} = \Gamma_1$

$P\,\Gamma_2\,P^{-1} = -\Gamma_2$, $T\,\Gamma_2\,T^{-1} = -\Gamma_2$

$P\,\Gamma_3\,P^{-1} = -\Gamma_3$, $T\,\Gamma_3\,T^{-1} = -\Gamma_3$

T symmetry : $T\,H(\mathbf{k})\,T^{-1} = H(-\mathbf{k}) \Rightarrow$ $d_1(\mathbf{k})$ even, $d_2(\mathbf{k})$, $d_3(\mathbf{k})$ odd functions

Kane-Mele model

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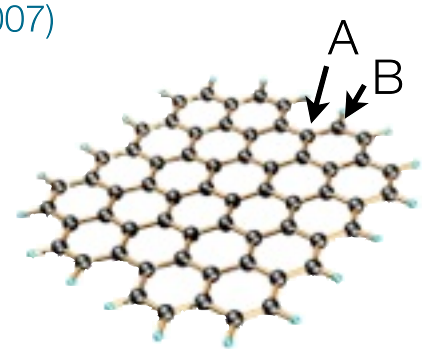

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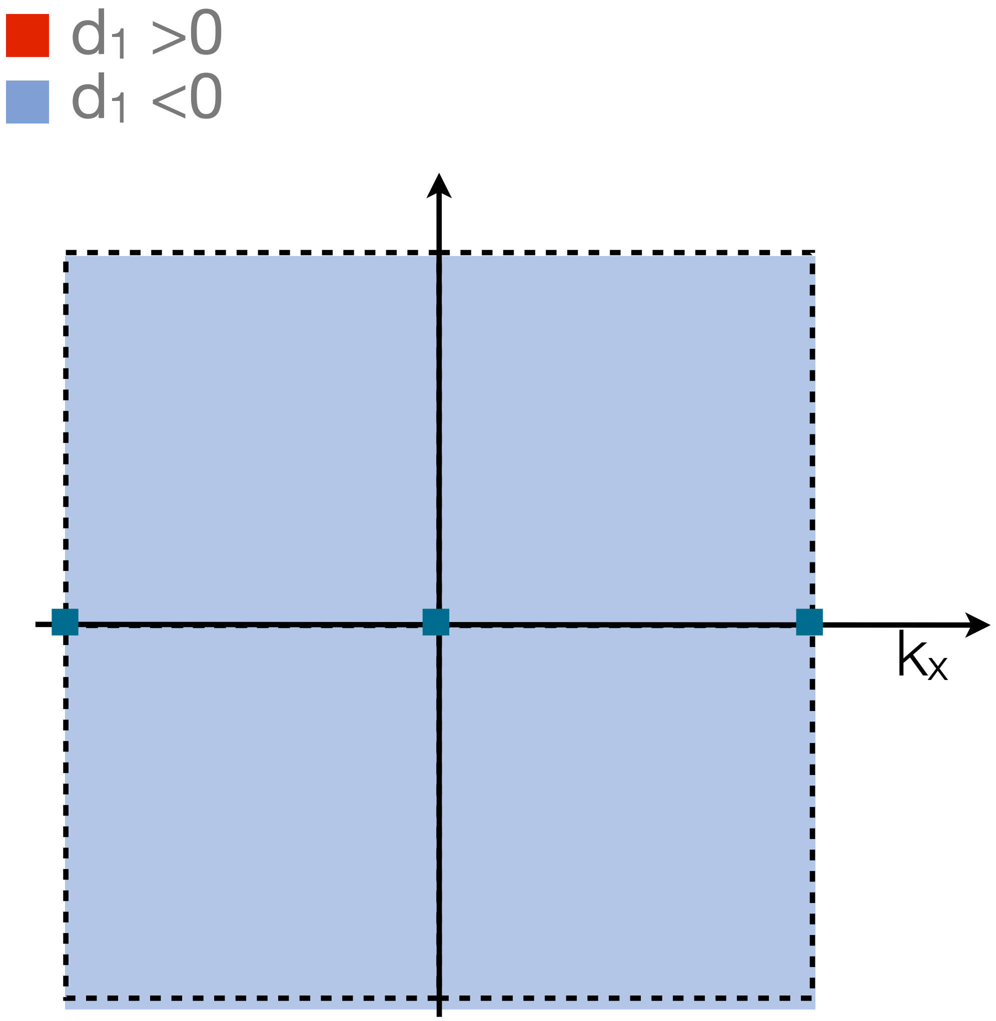

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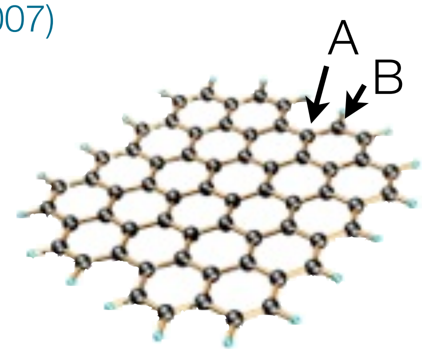

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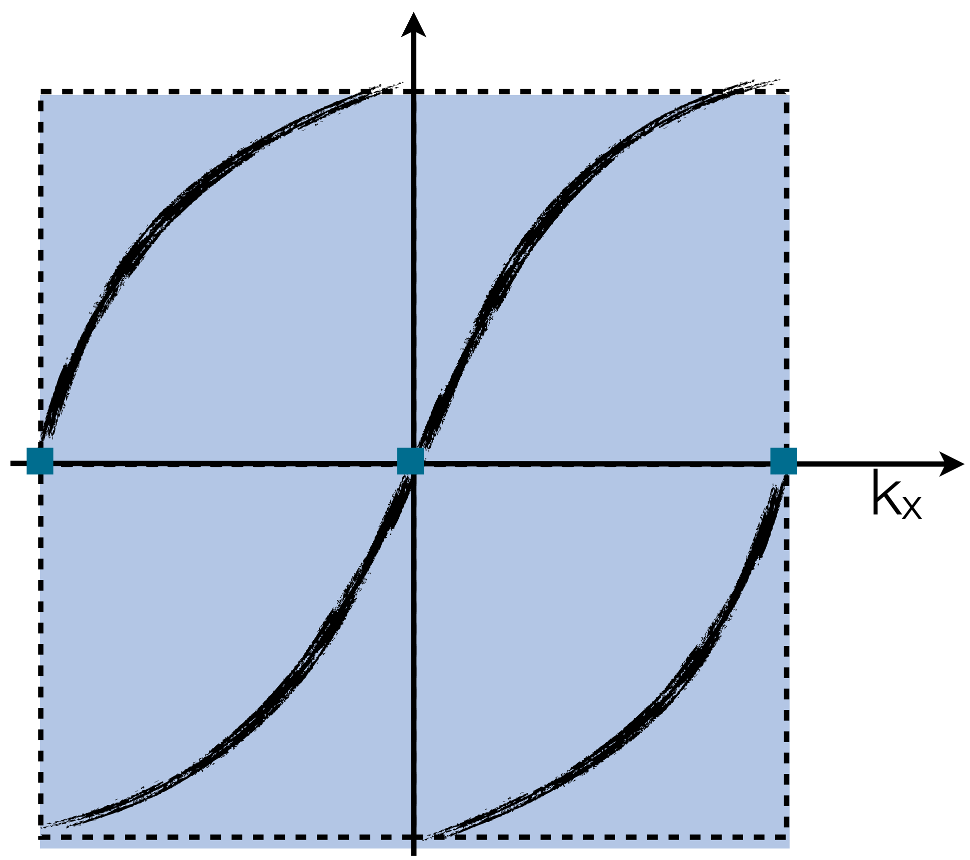
$d_1 < 0$



- d_2 has to vanish along lines connecting the Λ_i

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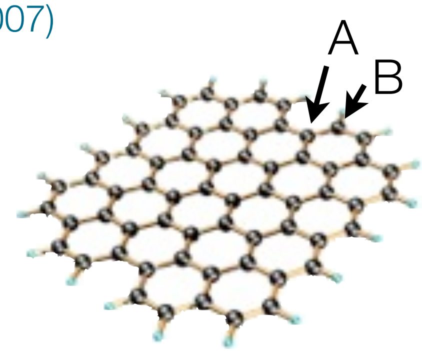

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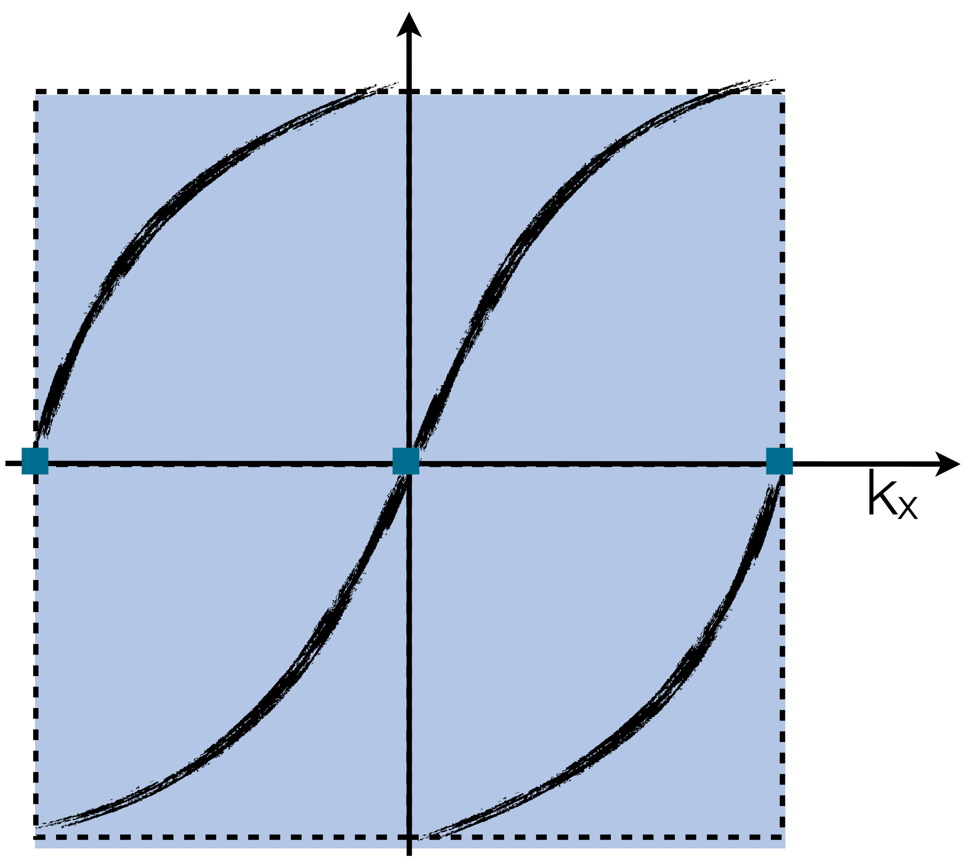

- d_2 has to vanish along lines connecting the Λ_i
- if d_1 uniform sign ⇒ no singularity

  ⇒ trivial topology (unique phase convention)

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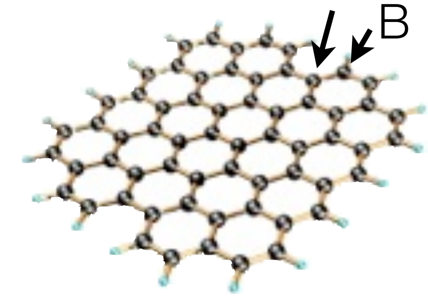

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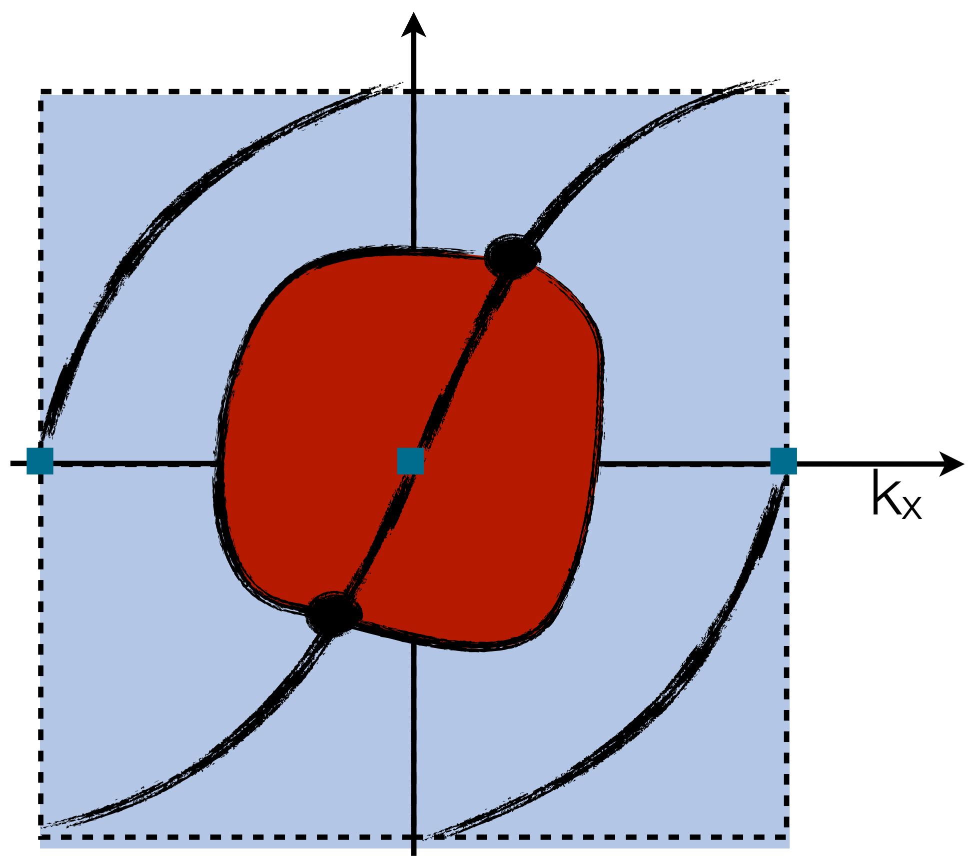

- d_2 has to vanish along lines connecting the Λ_i
- if d_1 uniform sign ⇒ no singularity

  ⇒ trivial topology (unique phase convention)
- if d_1 changes sign around 1 Λ_i

  ⇒ 2 singularities appear (for 1 phase convention)

  ⇒ twisted topology (obstruction)

Kane-Mele model

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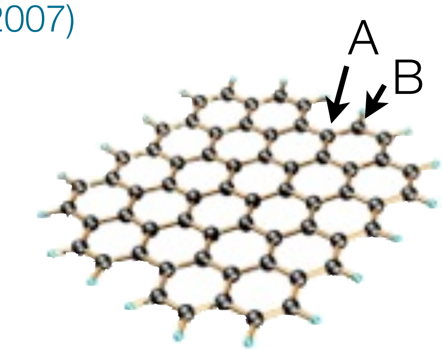

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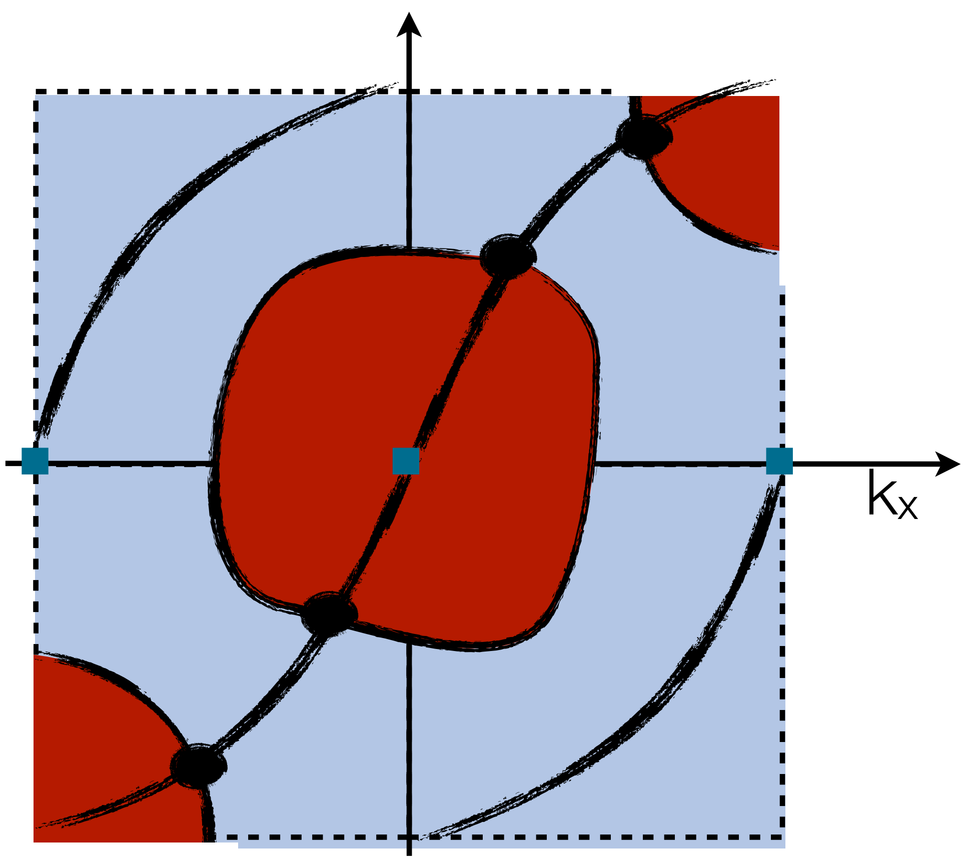

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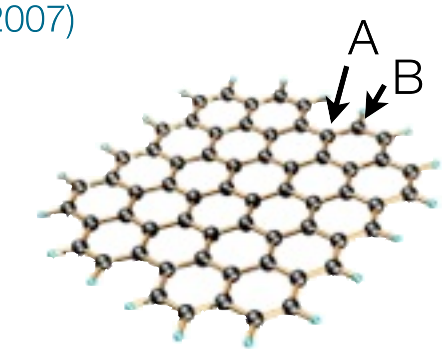
  ⇒ 2 singularities appear (for 1 phase convention)

  ⇒ twisted topology (obstruction)
- d_1 changes sign around 2 Λ_i

  ⇒ 4 singularities appear

Kane-Mele model

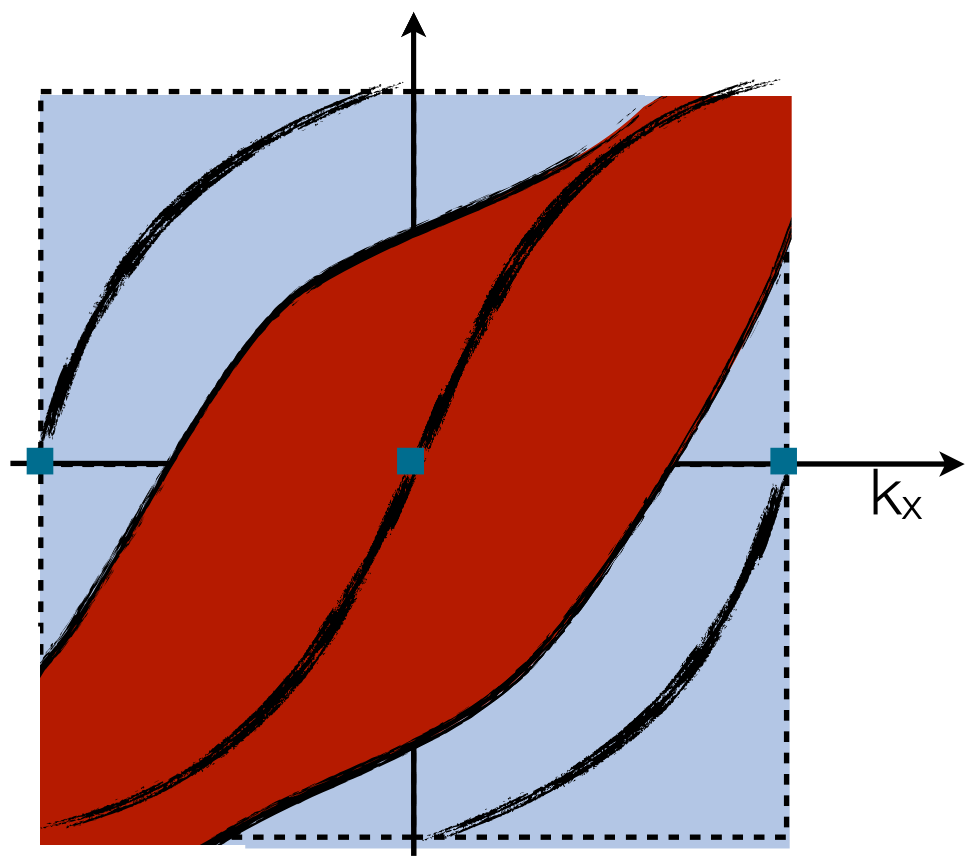
C.L.Kane and E.J.Mele PRL **95** (2005)
Fu, Kane, PRB **76** (2007)



Four Level System, two spin ½ ($\sigma \otimes S$) : $(A\uparrow, A\downarrow, B\uparrow, B\downarrow)$

- T symmetry ⇒ $d_1(\mathbf{k})$ even, $d_2(\mathbf{k})$, $d_3(\mathbf{k})$ odd functions
- eigenstates ill-defined for $d_1=d_2=0$

$d_1 > 0$
$d_1 < 0$



- d_2 has to vanish along lines connecting the Λ_i
- if d_1 uniform sign ⇒ no singularity

  ⇒ trivial topology (unique phase convention)
- if d_1 changes sign around 1 Λ_i

  ⇒ 2 singularities appear (for 1 phase convention)

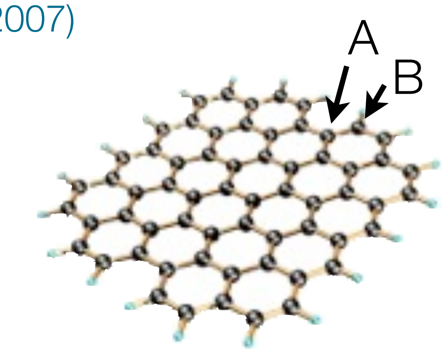
  ⇒ twisted topology (obstruction)
- d_1 changes sign around 2 Λ_i

  ⇒ 4 singularities appear, but can be removed

  ⇒ trivial topology

Kane-Mele model

C.L.Kane and E.J.Mele PRL **95** (2005)
Fu, Kane, PRB **76** (2007)



Four Level System, two spin ½ (σ ⊗ S) : $(A\uparrow, A\downarrow, B\uparrow, B\downarrow)$

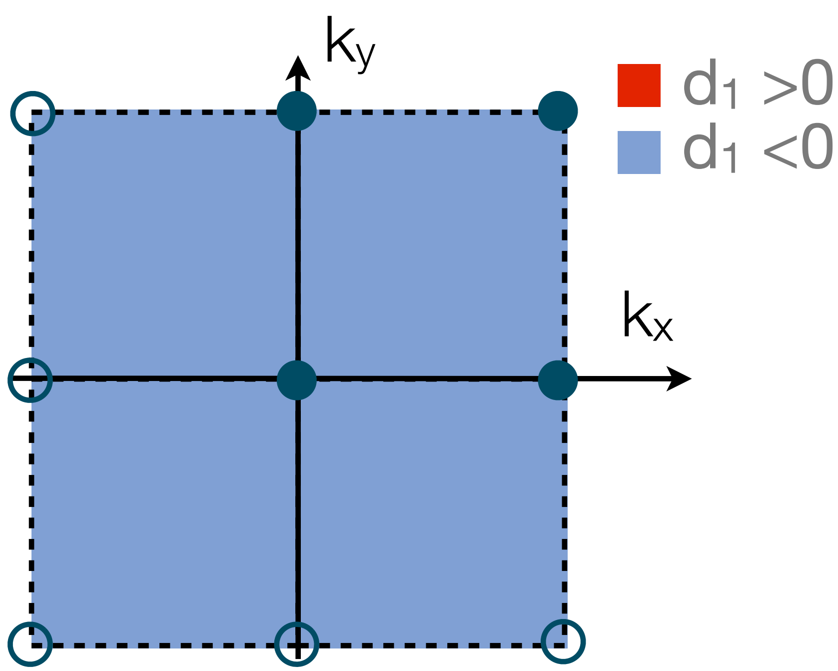
$$H(k) = d_1(k)\,\Gamma_1 + d_2(k)\,\Gamma_2 + d_3(k)\,\Gamma_3$$

Topological order ⟺ sign of d_1 at the Λ_i points

are filled bands mixing orthogonal states with ≠ parities ?

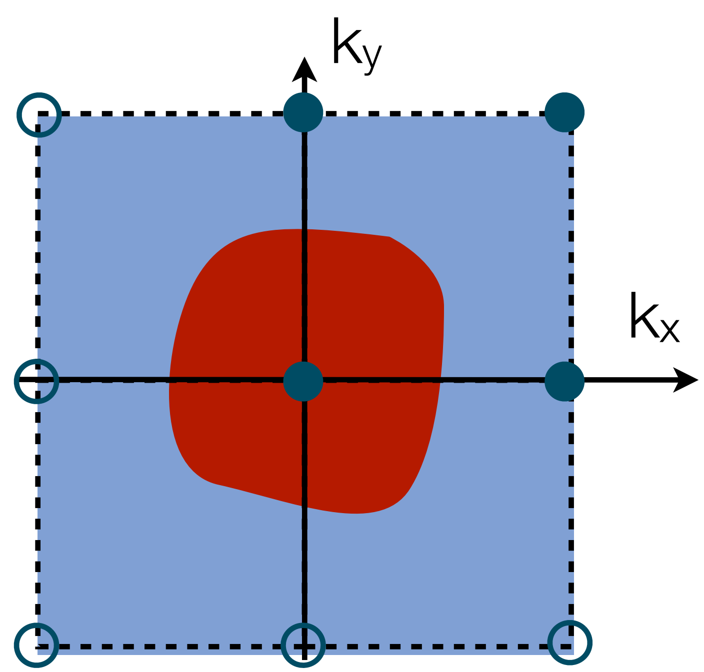
$$\prod_{i=1}^{4} d_1(\Lambda_i) > 0$$ trivial

$$\prod_{i=1}^{4} d_1(\Lambda_i) < 0$$ twisted



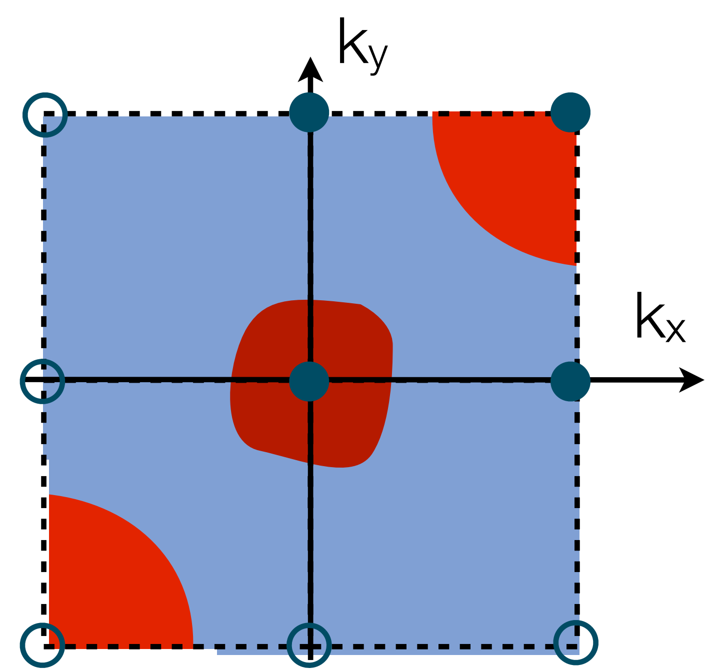
Trivial Insulator

(1parity in filled band)



Topological Insulator

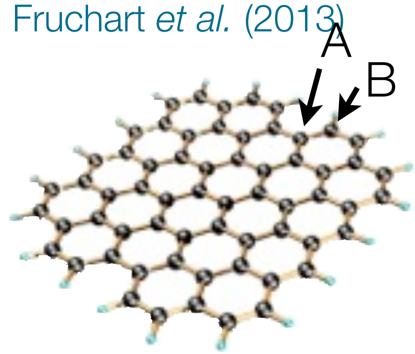
(mixing of parity in filled band)



Trivial Insulator

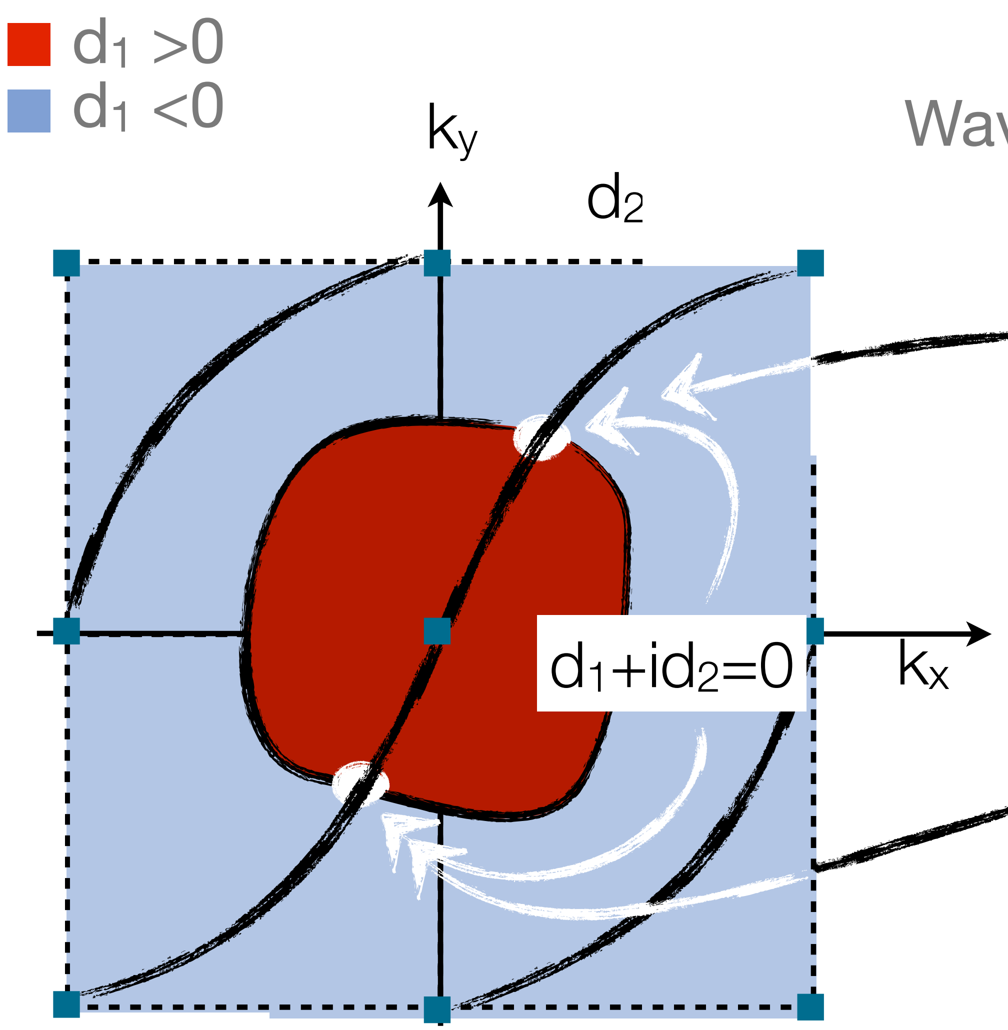
Kane-Mele model

Kane and Mele (1995)
Fruchart *et al.* (2013)



Four Level System, two spin ½ (σ ⊗ S) : $(A\uparrow, A\downarrow, B\uparrow, B\downarrow)$

Topological index : $\prod_{i=1}^{4} \mathrm{sgn}(d_1(\Lambda_i)) = (-1)^\nu$



Wavefunctions ill-defined for $d_1 + id_2 = te^{i\theta} \to 0$

$$|u_1^I\rangle \to \begin{pmatrix} 0 \\ -1 \\ 0 \\ 0 \end{pmatrix} \quad \text{and} \quad |u_1^{II}\rangle \to \begin{pmatrix} 0 \\ 0 \\ e^{i\theta} \\ 0 \end{pmatrix} \quad (d_3 > 0)$$

+ Berry monopole F^{II}

$$|u_1^I\rangle \to \begin{pmatrix} 0 \\ 0 \\ 0 \\ e^{i\theta} \end{pmatrix} \quad \text{and} \quad |u_1^{II}\rangle \to \begin{pmatrix} -1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \quad (d_3 < 0)$$

- Berry monopole F^{I}

Topological index : $\nu = \frac{C_I - C_{II}}{2} \mod 2$

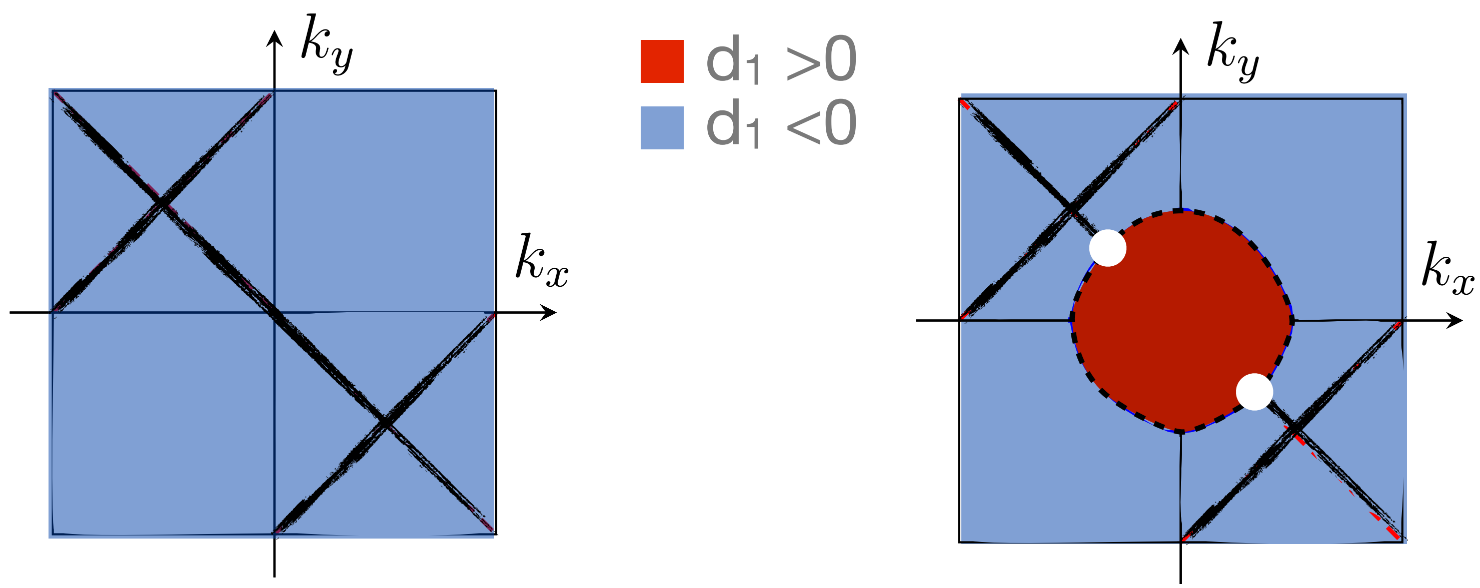
Kane-Mele topological invariant

Kane and Mele (1995)

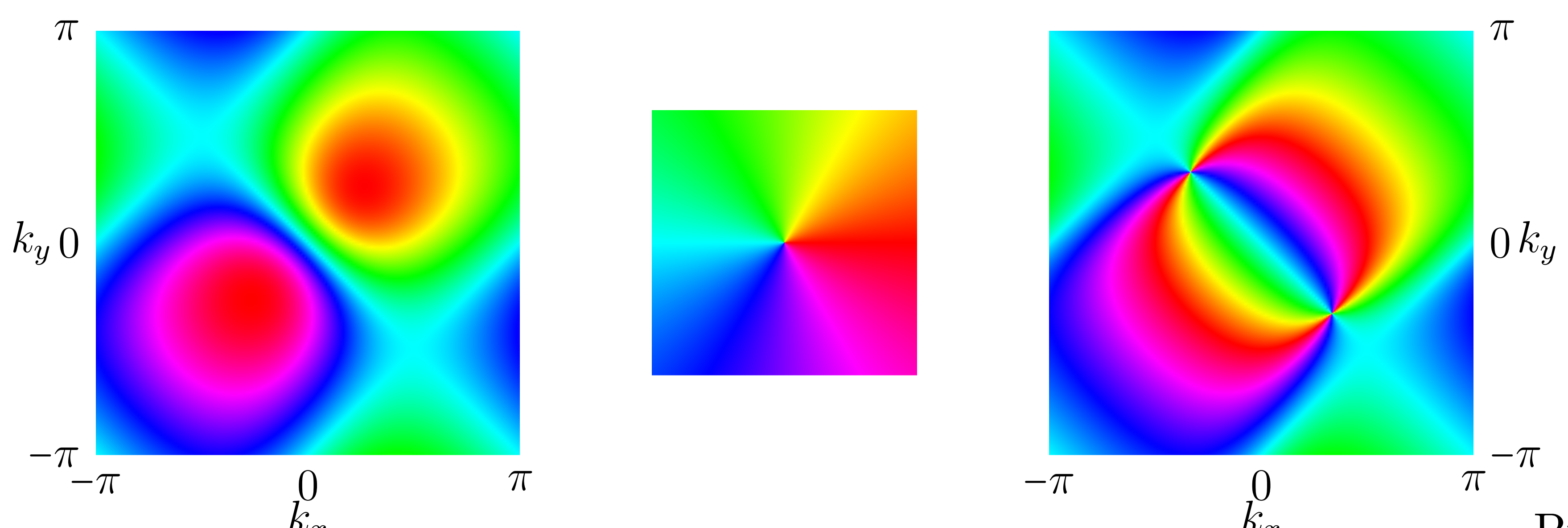
2Nx2N antisymmetric matrix : $m_{ij}(\mathbf{k}) = \langle u_i(\mathbf{k}) | T u_j(\mathbf{k}) \rangle$

Topological index ν : counts the parity of number of zeros of Pf(m)

$$\nu = \frac{1}{2\pi i} \oint_{\partial \mathrm{EBZ}} d \log \mathrm{Pf}(m) \mod 2$$



Wavefunctions ill-defined for $d_1 + i d_2 = t e^{i\theta} \to 0$



Phase of Pf(m)

$$\mathrm{Pf} m = \frac{d_1 (d_1 + i d_2)}{\sqrt{(d_1^2 + d_2^2)(d_1^2 + d_2^2 + d_5^2)}}$$

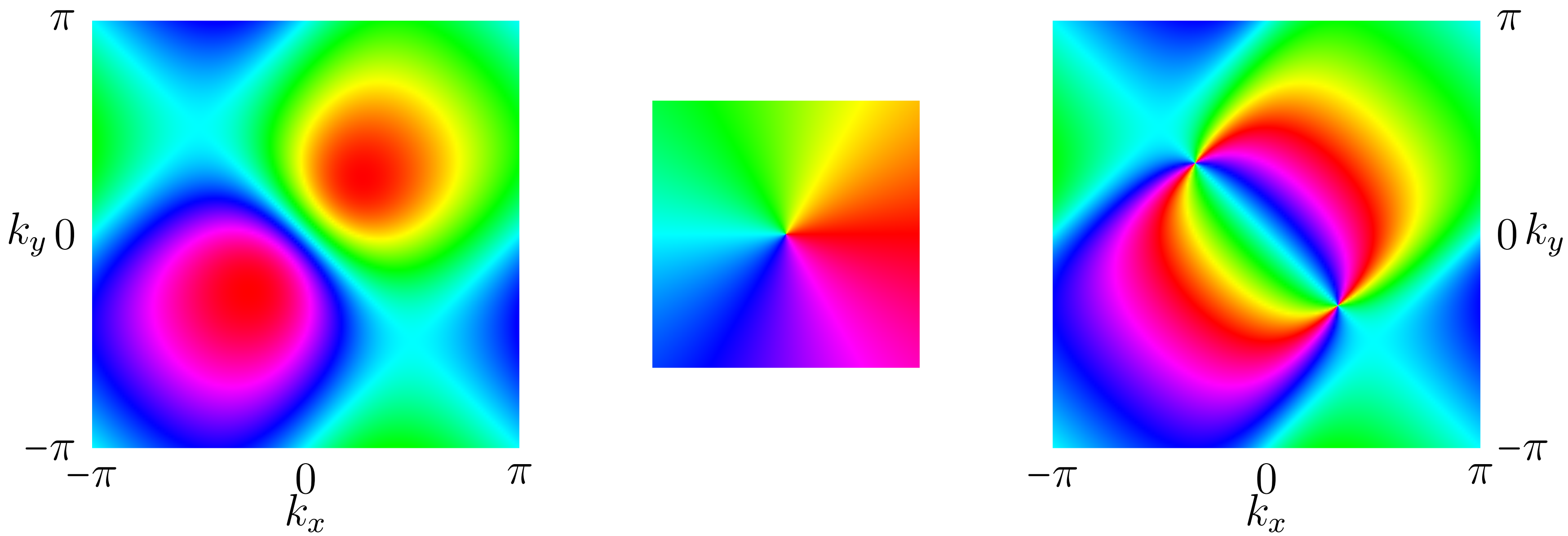
Kane-Mele topological invariant

Kane and Mele (1995)

2Nx2N antisymmetric matrix : $m_{ij}(\mathbf{k}) = \langle u_i(\mathbf{k}) | T u_j(\mathbf{k}) \rangle$

Topological index ν : counts the parity of number of zeros of Pf(m)

$$\nu = \frac{1}{2\pi i} \oint_{\partial \mathrm{EBZ}} d \log \mathrm{Pf}(m) \mod 2$$



Phase of Pf(m)

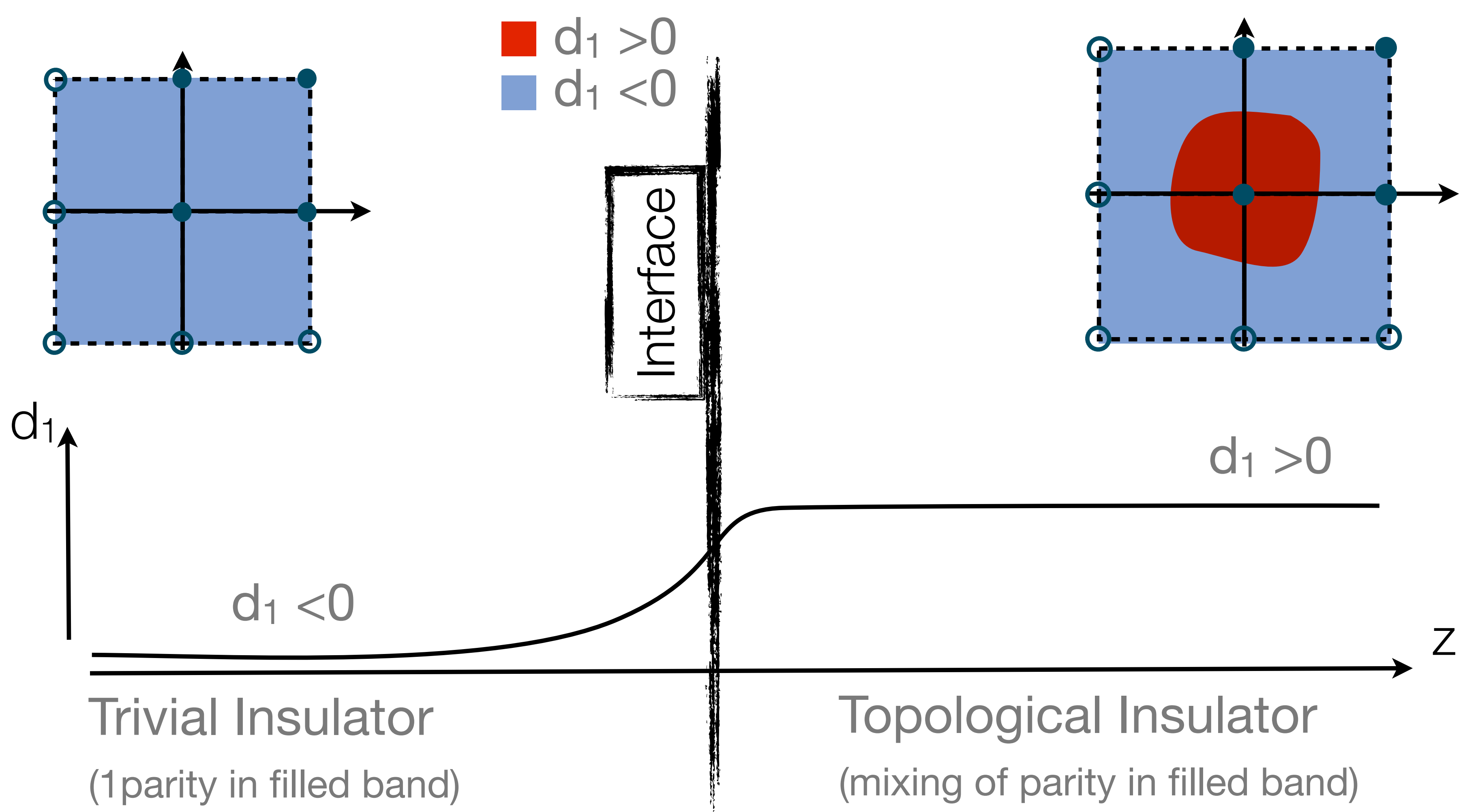
Topological index :

- if P and T symmetries : $\prod_{i=1}^{4} \mathrm{sgn}(d_1(\Lambda_i)) = (-1)^\nu$
- if I/II good spin quantum numbers $\nu = \dfrac{C_I - C_{II}}{2} \mod 2$

Kane-Mele model

Kane and Mele (1995)

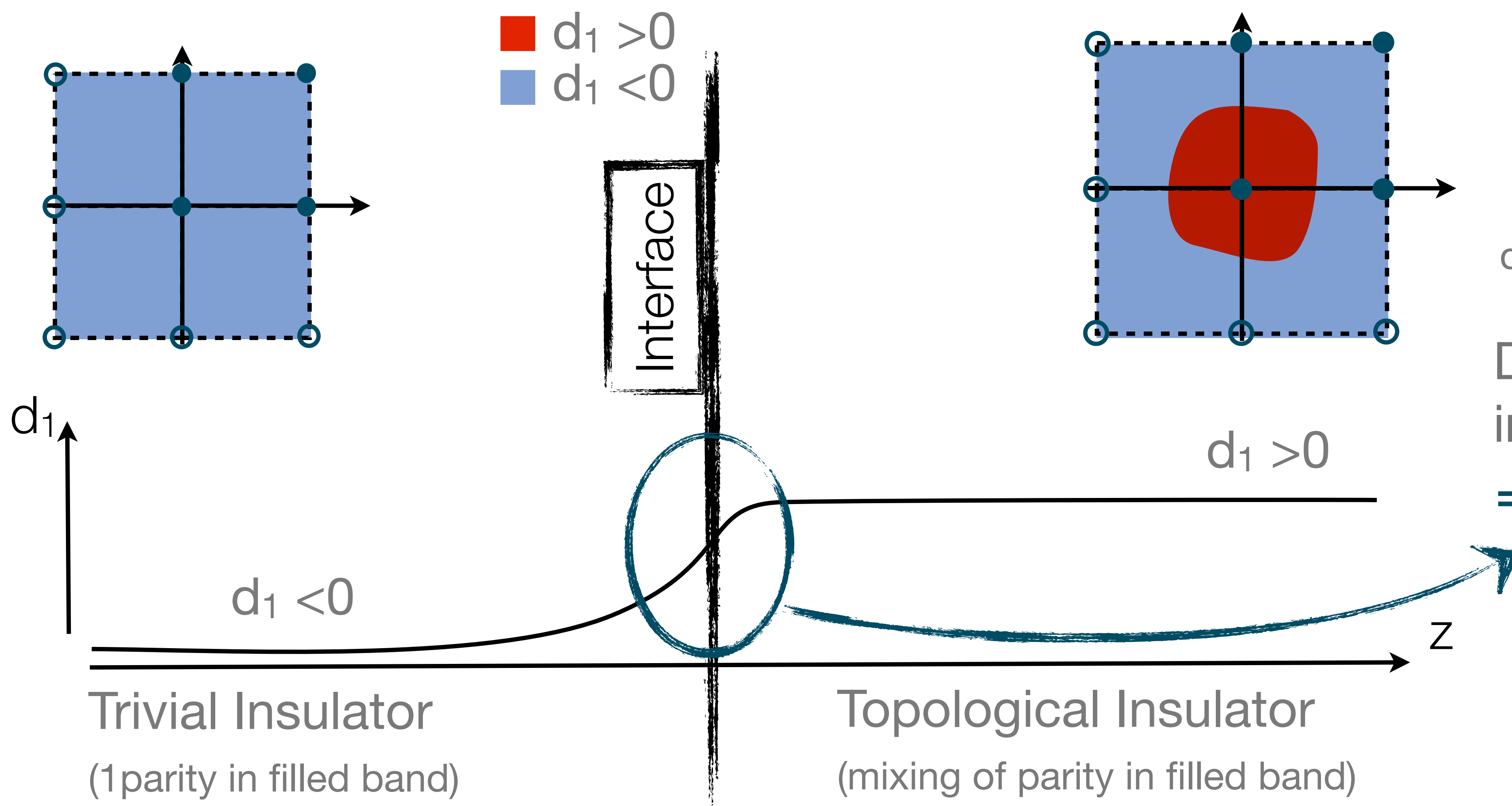
Topological order ⟺ sign of d_1 at the Λ_i points ⟺ surface states



Kane-Mele model

Kane and Mele (1995)

Topological order $\Longleftrightarrow$ sign of d_1 at the Λ_i points $\Longleftrightarrow$ surface states



$d_{i>1}(k)$~k around the Λ_0

Dirac eq. + mass (d_1) invertion

⇒ Dirac surface state

Bernevig-Hughes-Zhang model

Bernevig, Hughes, Zhang, Science 314 (2006)

(band inversion scenario)

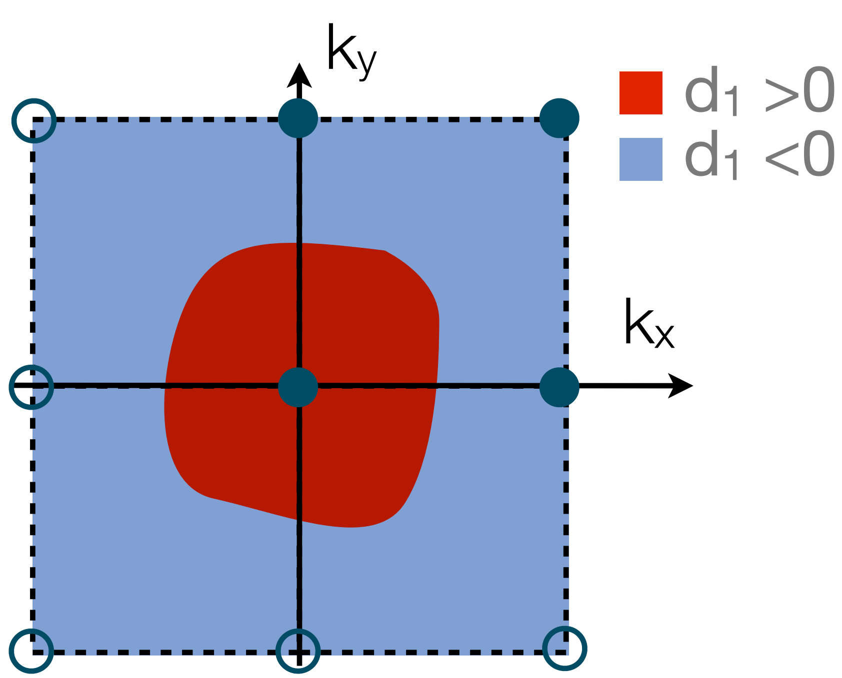
$$H(k) = d_1(k)\,\Gamma_1 \;+\; d_2(k)\,\Gamma_2 + d_3(k)\,\Gamma_3$$

Parity basis : $(s\uparrow, s\downarrow, p\uparrow, p\downarrow)$

$\Gamma_1 = \sigma_z \otimes I$ (diagonal operator)

$\Gamma_2 = \sigma_y \otimes I$, $\Gamma_5 = \sigma_x \otimes s_z$

d_1 is even around the Λ_i ($d_1(-\mathbf{k}) = d_1(\mathbf{k})$),
$d_{i>1}$ are odd around the Λ_i



Wavefunctions ill-defined at the Λ_i

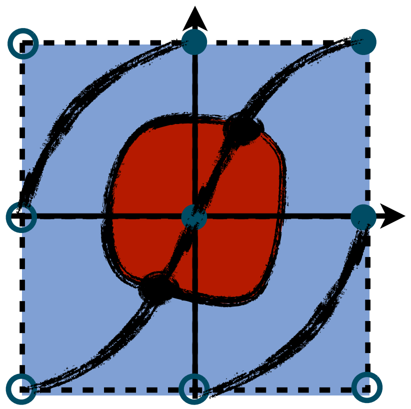
$$d_2 + i d_3 = t\, e^{i\theta}, t \to 0$$

$$|u_1^-\rangle \to \frac{1}{\mathcal{N}_1}\begin{pmatrix}0\\0\\0\\1\end{pmatrix} \quad \text{and} \quad |u_2^-\rangle \to \frac{1}{\mathcal{N}_2}\begin{pmatrix}0\\0\\1\\0\end{pmatrix} \qquad (d_1 > 0)$$

$$|u_1^-\rangle \to \frac{1}{\mathcal{N}_1}\begin{pmatrix}0\\ie^{-i\theta}\\0\\0\end{pmatrix} \quad \text{and} \quad |u_2^-\rangle \to \frac{1}{\mathcal{N}_2}\begin{pmatrix}ie^{-i\theta}\\0\\0\\0\end{pmatrix} \qquad (d_1 < 0)$$

Different singularities, but same topological order
⇒ necessity for a general definition of Z_2 topological order

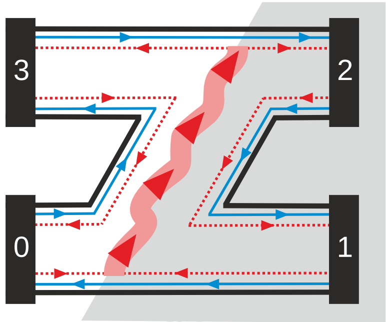
See K. Gawędzki talk

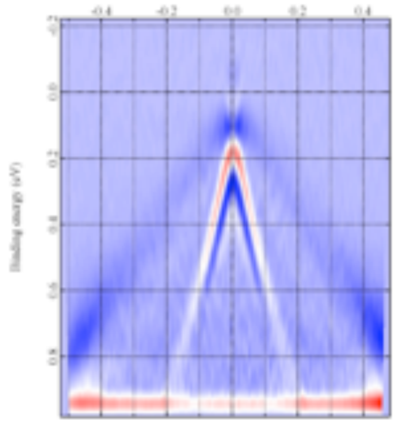


- Z$_2$ topological order from wavefunctions

  M. Fruchart, K. Gawedzki (ENS Lyon)

  Introduction to Topological Order in Insulators
  M. Fruchart, D. Carpentier and K. Gawedzki, CRAS (2013)





- Physical properties of Top. Ins. surfaces states

  C. Petitjean, E. Orignac, A. Fedorenko (ENS Lyon)

  Coll.: L. Lévy, T. Meunier (Néel Grenoble)

  Graphene-based heterojunction between two topological insulators
  O. Shevtsov, *et al.*, Phys. Rev. X **2**, 031004 (2012)

  Tunable thermopower in a graphene-based topological insulator
  O. Shevtsov, et al., Phys. Rev. B **85**, 245441 (2012)

  Topological surface states of strained Mercury-Telluride probed by ARPES
  O. Crauste, *et al.*, arXiv:1307.2008

Support : ANR IsoTop/2010 and ANR SemiTopo/2012

Thank you for your attention