

6. TR invariant topological band-structures (topological insulators)

15 years after Haldane's model and more than 20 years after the QHE, Kane and Mele realized that topologically non-trivial insulators exist where Time reversal symmetry is not broken

C.L. Kane, E.J. Mele Phys. Rev. Lett. 95, 226801 (2005)

This type of models can be described by a second type of invariant, a $\mathbb{Z}_2$ invariant with two values

The Kane-Mele model arises from a doubling of the Haldane model including a spin degree of freedom and in general spin-orbit coupling

Before discussing this model we want to see how the spin degree can make topological bulk transport possible in TR symmetric systems.

6.1 Topological spin pump

A simple TR symmetric spin pump was suggested by Fu and Kane in Phys. Rev. B 74, 195312 (2006). Consider two copies of a Kane-Mele model for

Spin up $\uparrow$ and spin $\downarrow$ with 4×4 momentum Hamiltonian

$$(279) \quad \underline{h}(k) = \begin{bmatrix} \Delta_{\uparrow} & -t_1 - t_2 e^{-ik} & 0 & 0 \\ -t_1 - t_2 e^{ik} & -\Delta_{\uparrow} & 0 & 0 \\ 0 & 0 & \Delta_{\downarrow} & -t_1 - t_2 e^{-ik} \\ 0 & 0 & -t_1 - t_2 e^{ik} & -\Delta_{\downarrow} \end{bmatrix}$$

Now choose

$$(280) \quad \begin{aligned} \Delta_{\uparrow}(t) &= -\Delta_{\downarrow}(t) = \Delta \sin(t/T) \\ t_{1,2}(t) &= t_0 (1 \pm \varepsilon \cos(t/T)) \end{aligned}$$

TR symmetry: here spin! and 1+1 dimension
 (k, t)

$$T = i \underline{\partial}_g k$$

$$(281) \quad \sigma_y \underline{h}^*(-k, -t) \sigma_y \stackrel{?}{=} \underline{h}(k, t)$$

$$\begin{bmatrix} 0 & -\mathbb{I}_{2 \times 2} \\ \mathbb{I}_{2 \times 2} & 0 \end{bmatrix} \begin{bmatrix} h_{\uparrow}^*(-k, -t) & 0 \\ 0 & h_{\downarrow}^*(-k, -t) \end{bmatrix} \begin{bmatrix} 0 & -\mathbb{I}_{2 \times 2} \\ \mathbb{I}_{2 \times 2} & 0 \end{bmatrix}$$

$$(282) \quad = \begin{bmatrix} -h_{\downarrow}^*(-k, -t) & 0 \\ 0 & -h_{\uparrow}^*(-k, -t) \end{bmatrix} \stackrel{?}{=} \begin{bmatrix} h_{\uparrow}(k, t) & 0 \\ 0 & h_{\downarrow}(k, t) \end{bmatrix}$$

For this we note

$$(283) \quad h_{\uparrow}(k, t) = \Delta_{\uparrow} \phi_z - (t_1 + t_2 \cos k) \phi_x - t_2 \sin k \phi_y$$

$$h_{\downarrow}(k, t) = \Delta_{\downarrow} \phi_z - (t_1 + t_2 \cos k) \phi_x - t_2 \sin k \phi_y$$

$$(284) \quad \Delta_{\uparrow, \downarrow}(-t) = -\Delta_{\uparrow, \downarrow}(t)$$

$$t_{1,2}(-t) = t_{1,2}(t)$$

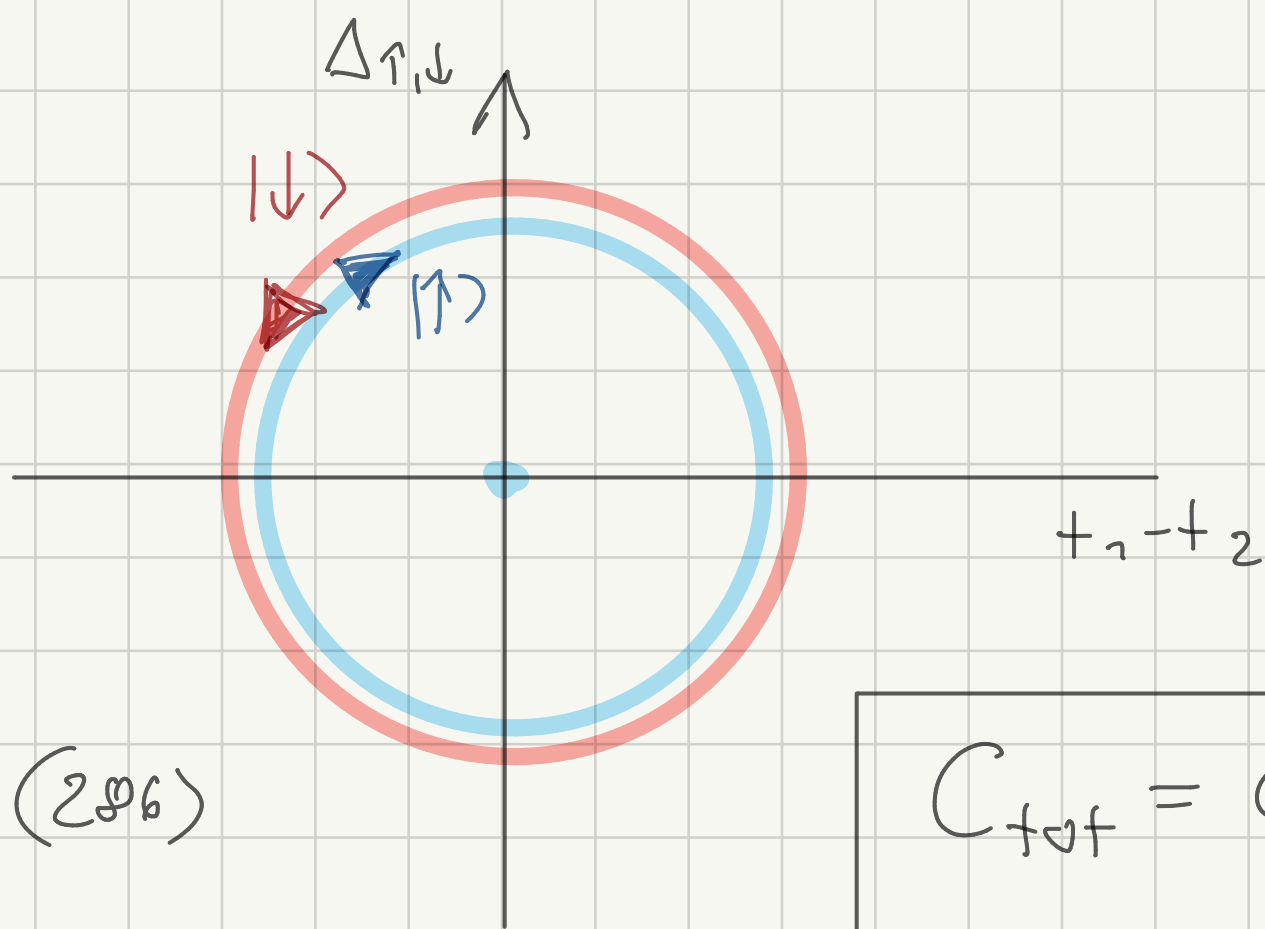
so

$$(285) \quad \begin{aligned} h_{\uparrow}^*(-k, -t) &= -\Delta_{\uparrow}(t) \phi_z \\ &\quad - (t_1(t) + t_2(t) \cos k) \phi_x - t_2(t) \sin k \phi_y \\ &= h_{\downarrow}(k, t) \end{aligned}$$

and

$$h_{\downarrow}^*(-k, -t) = h_{\uparrow}(k, t)$$

$\Rightarrow$ TR symmetry!



$$C_{\uparrow} = +1$$

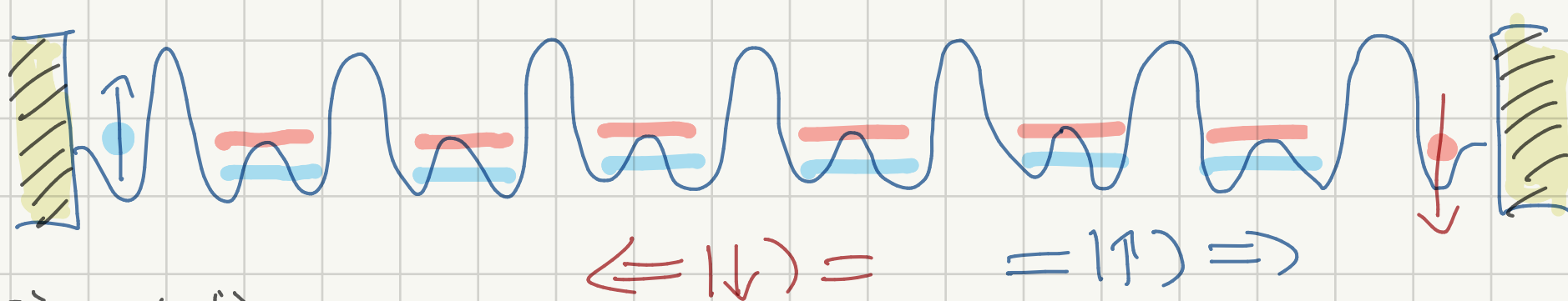
$$C_{\downarrow} = -1$$

(206)

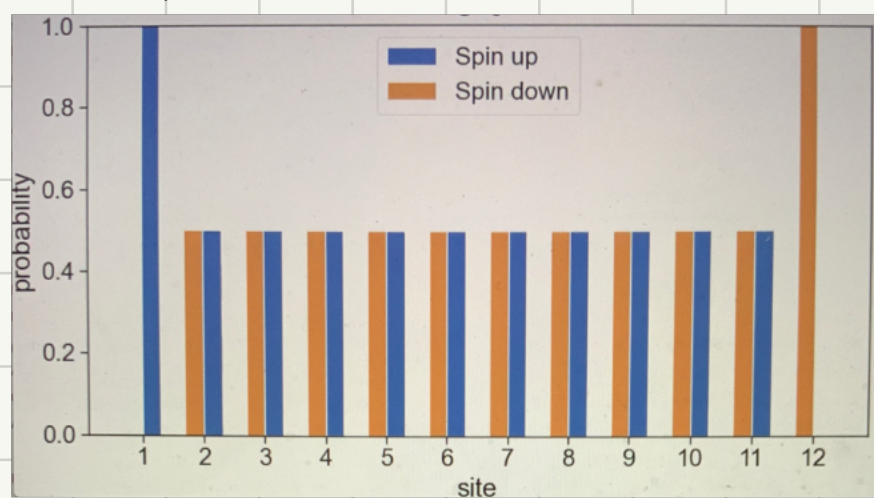
$$C_{\text{tot}} = C_{\uparrow} + C_{\downarrow} = 0$$

as expected from TR symmetry

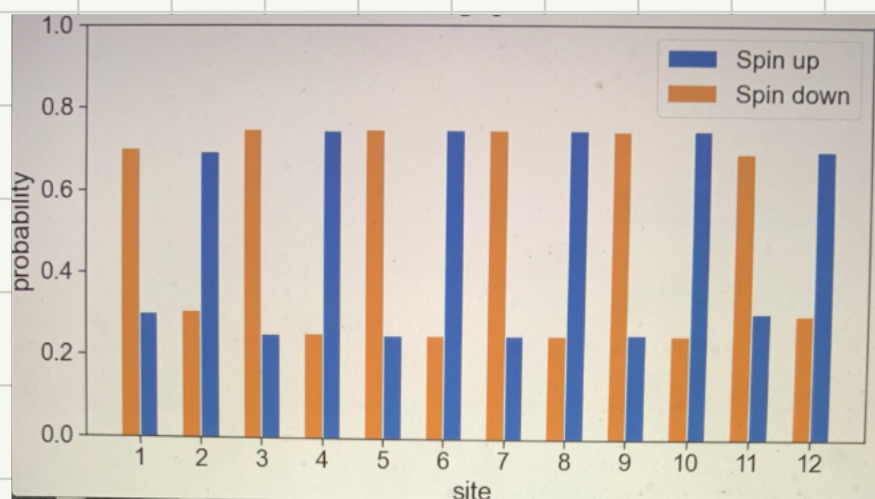
No net transport of charge, but spin pump



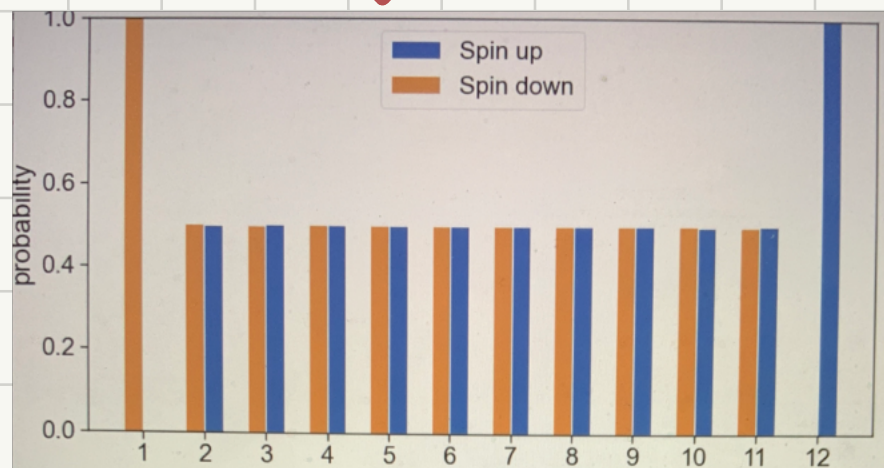
Simulation



$t=0$



$t=T$



There is a topological quantum number

(287)

$$\nu_2 = \frac{1}{2} |C_{\uparrow} - C_{\downarrow}|$$

which is a $\mathbb{Z}_2$ topological index

This model is however over-simplified as it does not allow for spin coupling. If there is spin-orbit coupling the individual Chern numbers $C_{\uparrow}$ and $C_{\downarrow}$ are no longer good quantum numbers but there is still a proper $\mathbb{Z}_2$ topological invariant.

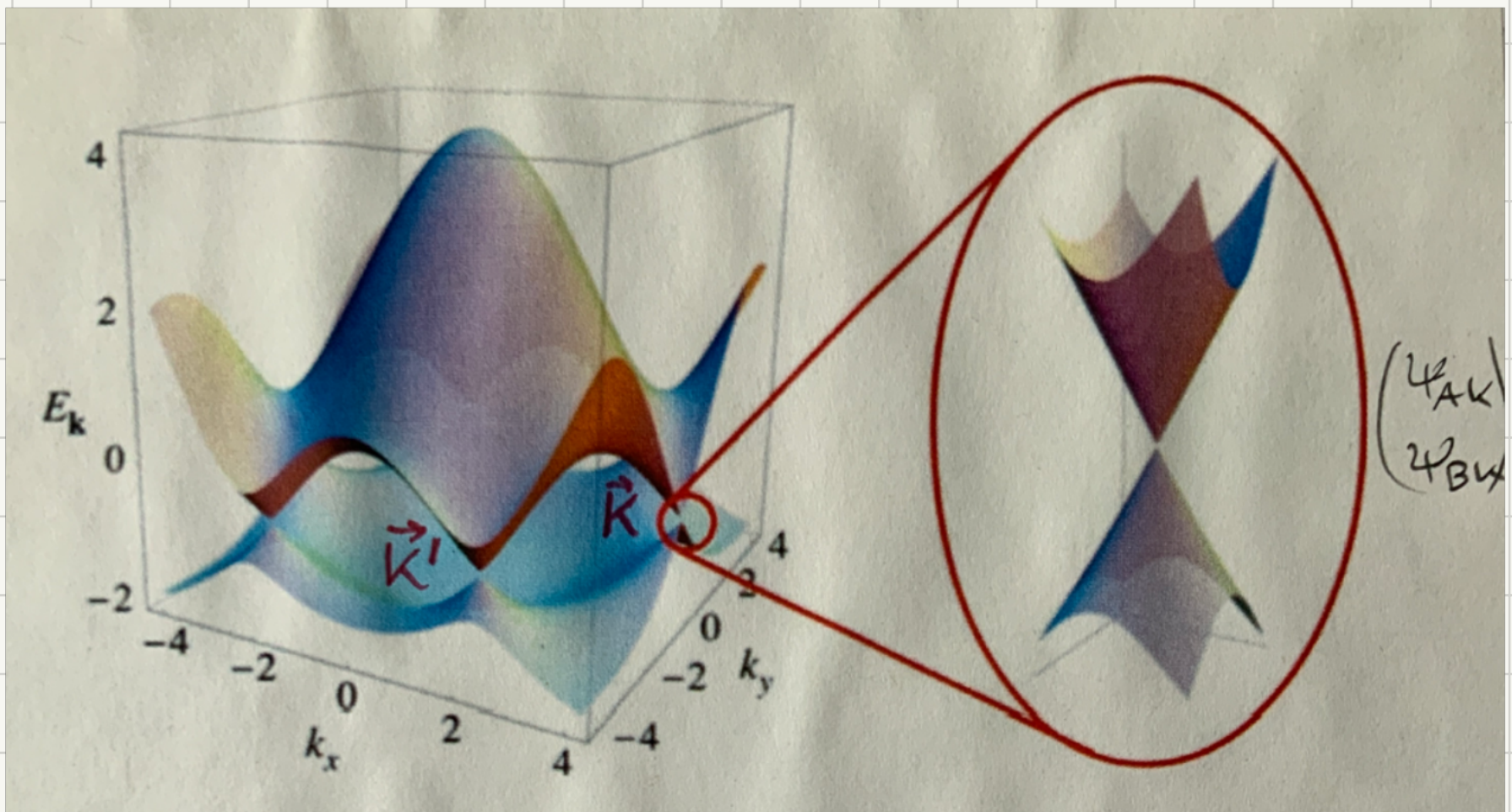
6.2 Continuum version of Kane-Mele model

We now want to discuss the 2D Kane-Mele model, starting with a conceptually simpler continuum version arising from the low-energy limit of Graphene (265)

$$(288) \quad \begin{aligned} \underline{h}(\vec{k} + \delta\vec{k}) &= -\frac{3}{2}t_1(\delta k_x \underline{\sigma}_x + \delta k_y \underline{\sigma}_y) \\ \underline{h}(\vec{k}' + \delta\vec{k}) &= -\frac{3}{2}t_1(-\delta k_x \underline{\sigma}_x + \delta k_y \underline{\sigma}_y) \end{aligned}$$

We now introduce an effective model which treats the Dirac fermions at $\vec{k}$ and $\vec{k}'$ as independent species

$\Rightarrow$ 4-component state



$$(289) \quad \hat{\psi} = (\hat{\psi}_{AK}, \hat{\psi}_{BK}, \hat{\psi}_{AK'}, \hat{\psi}_{BK'})$$

and introduce the real-space Hamiltonian

$$(290) \quad H_0 = -i\hbar v_F \hat{\psi}^\dagger(\vec{r}) [\sigma_x \tau_z \partial_x + \sigma_y \partial_y] \hat{\psi}(\vec{r})$$

• σ_x, σ_y Pauli matrices in (ψ_{AK}, ψ_{BK})
and $(\psi_{AK'}, \psi_{BK'})$

$$\tau_z = \begin{pmatrix} \mathbb{I}_2 & 0 \\ 0 & -\mathbb{I}_2 \end{pmatrix} \quad \begin{matrix} \leftarrow K \\ \leftarrow K' \end{matrix}$$

$$v_F = -\frac{3}{2} \alpha t_1$$

in matrix form

$$(291) \quad H_0 = -i\hbar v_F \begin{pmatrix} \hat{\psi}^\dagger \\ \hat{\psi} \end{pmatrix} \begin{bmatrix} \partial_x \partial_x + \partial_y \partial_y & 0 \\ 0 & -\partial_x \partial_x + \partial_y \partial_y \end{bmatrix} \begin{pmatrix} \hat{\psi} \\ \hat{\psi} \end{pmatrix}$$

Now lets add electron spin

$\hat{\psi} \rightarrow$ 2 components

and spin-orbit coupling

$$(292) \quad H_{SO} = \lambda_{SO} \begin{pmatrix} \hat{\psi}^\dagger \\ \hat{\psi} \end{pmatrix} \underbrace{\partial_z}_{\substack{\text{A,B space} \\ \nearrow}} \underbrace{\tau_z}_{\substack{\uparrow \\ \text{K,u' space}}} \underbrace{S_z}_{\nwarrow \text{Spin}} \begin{pmatrix} \hat{\psi} \\ \hat{\psi} \end{pmatrix}$$

Remarks:

- H_{SO} conserves TR symmetry
- H_{SO} is only allowed generalization to preserve inversion $z \leftrightarrow -z$
- H_{SO} opens a gap
 $\Rightarrow$ insulator!

Kane-Mele model (continuum)

$$(293) \quad H = -i\hbar v_F \begin{pmatrix} \hat{\psi}^\dagger \\ \hat{\psi} \end{pmatrix} (\partial_x \tau_z \partial_x + \partial_y \partial_y) \begin{pmatrix} \hat{\psi} \\ \hat{\psi} \end{pmatrix} + \lambda_{SO} \begin{pmatrix} \hat{\psi}^\dagger \\ \hat{\psi} \end{pmatrix} S_z \partial_z \tau_z \begin{pmatrix} \hat{\psi} \\ \hat{\psi} \end{pmatrix}$$

6.3 Kane Mele model on a lattice

Now we want to generalize the low-energy Hamiltonian (293) to a full lattice model

$$(294) \quad H = t_1 \sum_{\langle ij \rangle, \sigma} \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + i\lambda_{so} \sum_{\langle\langle ij \rangle\rangle, \sigma, \sigma'} v_{ij} \hat{c}_{i\sigma}^\dagger S_{\sigma\sigma'}^z \hat{c}_{j\sigma'}$$

- first term corresponds to Graphene with isotropic hopping to nearest neighbors NN
- Second term is next nearest neighbor NNN hopping with spin dependent sign

$$\langle ij \rangle : \text{NN} \quad \langle\langle ij \rangle\rangle : \text{NNN}$$

$$v_{ij} = \pm 1 \text{ as in Haldane}$$

For $\lambda \approx 0$ the lattice Hamiltonian reduces to (293)

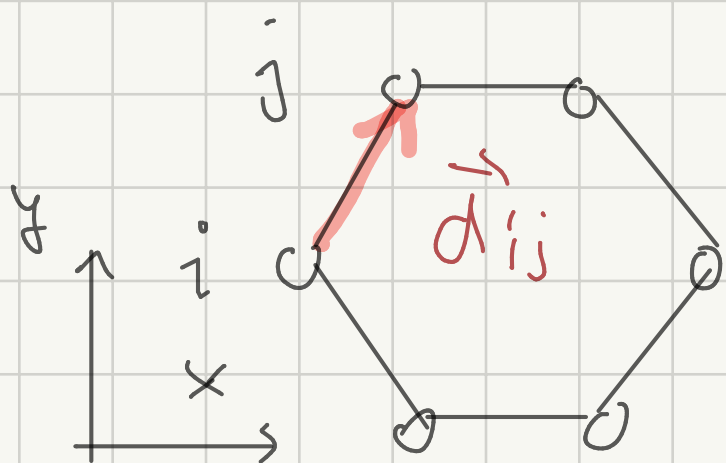
generalized spin-orbit coupling & spin mixing

(294) conserves the spin projection in z direction. One can however add a more general spin-orbit coupling (SOC) term

Rashba spin-orbit coupling

$$(295) \quad H_R = i\lambda_R \sum_{\langle ij \rangle} \hat{c}_{i0}^\dagger \left[(\vec{\hat{S}} \times \vec{d}_{ij})_z \right]_{00'} \hat{c}_{j0'}$$

where $\vec{d}_{ij}$ is the vector connecting the lattice sites i and j

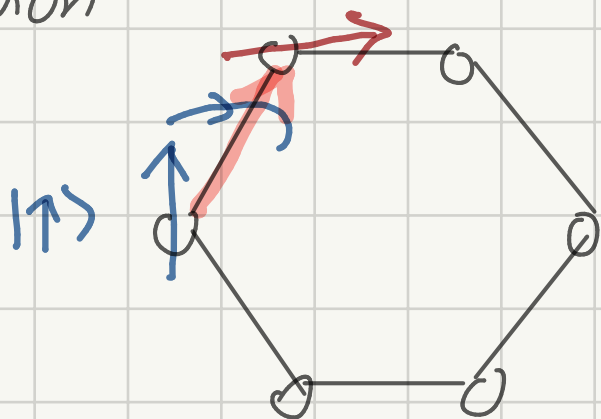


$$\text{since } \vec{d}_{ij} = \alpha \vec{e}_x + \beta \vec{e}_y$$

$$\Rightarrow (\vec{\hat{S}} \times \vec{d}_{ij})_z \sim \hat{S}_x \text{ and } \hat{S}_y$$

$\Rightarrow$ spin projection in z
no longer conserved

Rashba SOC rotates the spin upon hopping of the electron



For $\varepsilon \neq 0$ H_R can be written in momentum space as

$$(296) \quad h_R(\vec{k} + \delta\vec{k}) = \sigma_x \hat{S}_y - \sigma_y \hat{S}_x$$

$$h_R(\vec{k}' + \delta\vec{k}) = -\sigma_x \hat{S}_y - \sigma_y \hat{S}_z$$

(remember: σ_x, σ_y act in A, B sublattice space)

Inversion breaking

Another term that can be added is one that breaks inversion symmetry

(297)

$$H_I = \lambda_I \sum_{j,b} \varepsilon_j \hat{C}_{jb}^\dagger \hat{C}_{jb}$$

$\varepsilon_j = \pm 1$
for A, B
sublattice

Combining these terms gives the most general form of the Kane Mele model

$$H_{KM} = t \sum_{\langle ij \rangle} \hat{C}_i^\dagger \hat{C}_j + i\lambda_{so} \sum_{\langle\langle ij \rangle\rangle} v_{ij} \hat{C}_i^\dagger \hat{S}^z \hat{C}_j \\ + i\lambda_R \sum_{\langle ij \rangle} \hat{C}_i^\dagger (\hat{\vec{S}} \times \hat{\vec{d}}_{ij})_z \hat{C}_j + \lambda_I \sum_j \varepsilon_j \hat{C}_j^\dagger \hat{C}_j$$

(298) (summation over spin indices is implicit)

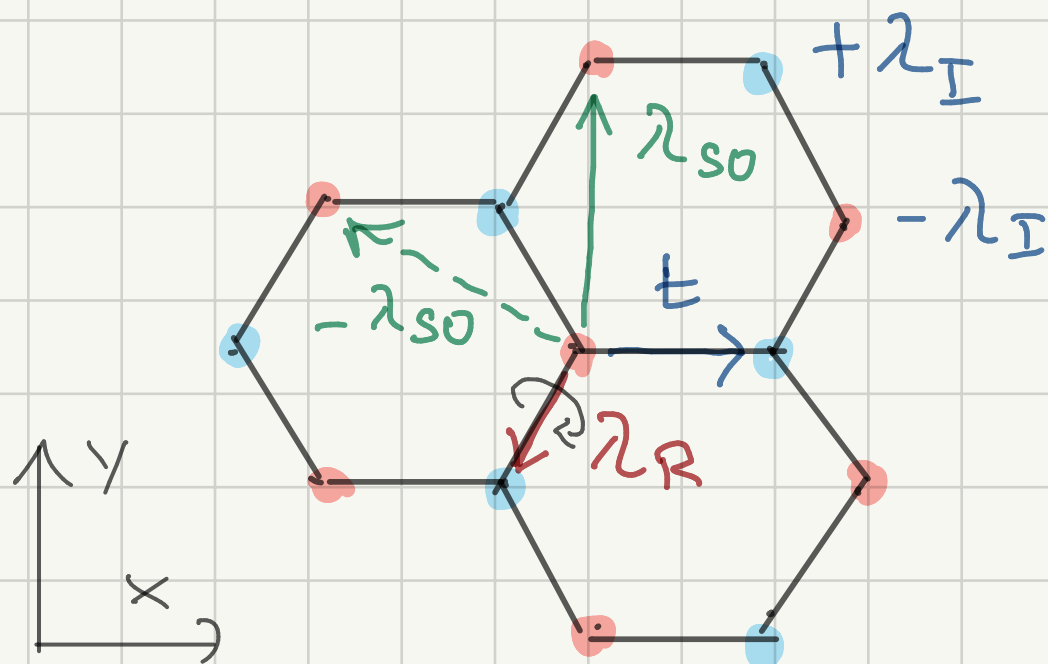
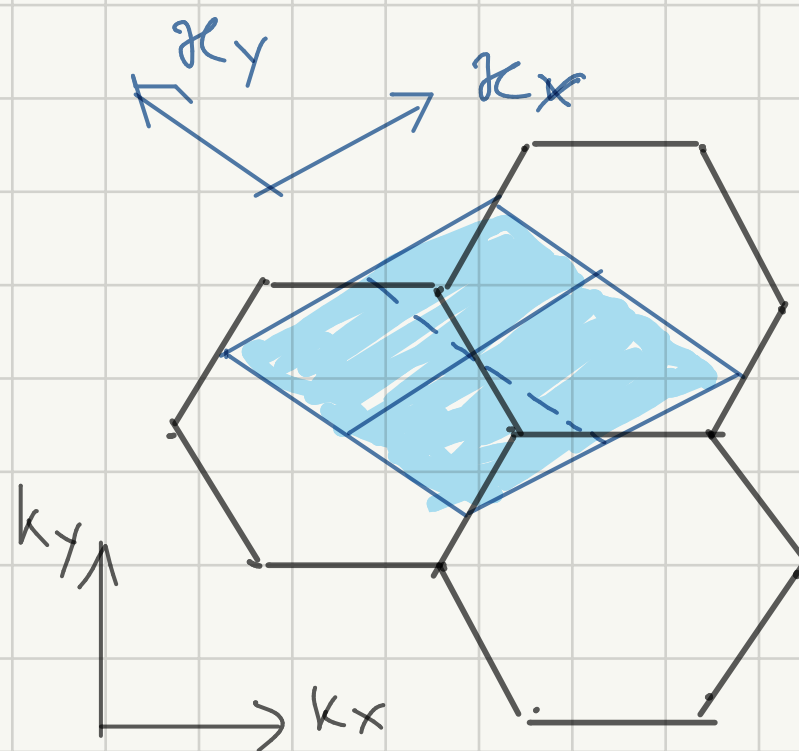


illustration of
processes



Brillouin zone

Transforming into momentum space we get a 4×4 matrix for 2 spin degrees and 2 sublattices

$$(299) \quad H_{KM} = \sum_{\vec{b}} \hat{C}^\dagger(\vec{b})^T \underline{h}_{KM}(\vec{b}) \hat{C}(\vec{b})$$

where $\hat{C}(\vec{b}) = (\hat{C}_{A\uparrow}, \hat{C}_{B\uparrow}, \hat{C}_{A\downarrow}, \hat{C}_{B\downarrow})^T$

$$(300) \quad \underline{h}_{KM}(\vec{b}) = \begin{pmatrix} d_{SO\uparrow} & d_t & 0 & \bar{d}_R \\ d_t^* & -d_{SO\uparrow} & d_R & 0 \\ 0 & d_R^* & d_{SO\downarrow} & d_t \\ \bar{d}_R^* & 0 & d_t^* & -d_{SO\downarrow} \end{pmatrix} \begin{matrix} \left. \begin{matrix} \text{---} \\ \text{---} \end{matrix} \right\} \uparrow \uparrow \\ \left. \begin{matrix} \text{---} \\ \text{---} \end{matrix} \right\} \downarrow \downarrow \end{matrix}$$

where

$$d_{SO\uparrow,\downarrow} = \lambda_{\pm} \pm d_{15}$$

$$d_t = d_4 + i d_{12}$$

(301)

$$\bar{d}_R = -(d_4 + d_{23}) - i(d_3 - d_{24})$$

$$d_R = (d_4 - d_{23}) + i(d_3 + d_{24})$$

and

$$d_R, \bar{d}_R \sim \lambda_R$$

$$d_1 = t(1 + \lambda \cos x \cos y)$$

$$d_3 = \lambda_R (1 - \cos x \cos y)$$

$$d_4 = -\sqrt{3} \lambda_R \sin x \sin y$$

$$d_{12} = -2t \cos x \sin y$$

$$(302) \quad d_{15} = \lambda_{SO} (2 \sin 2x - 4 \sin x \cos y)$$

$$d_{23} = -\lambda_R \cos x \sin y$$

$$d_{24} = \sqrt{3} \lambda_R \sin x \cos y$$

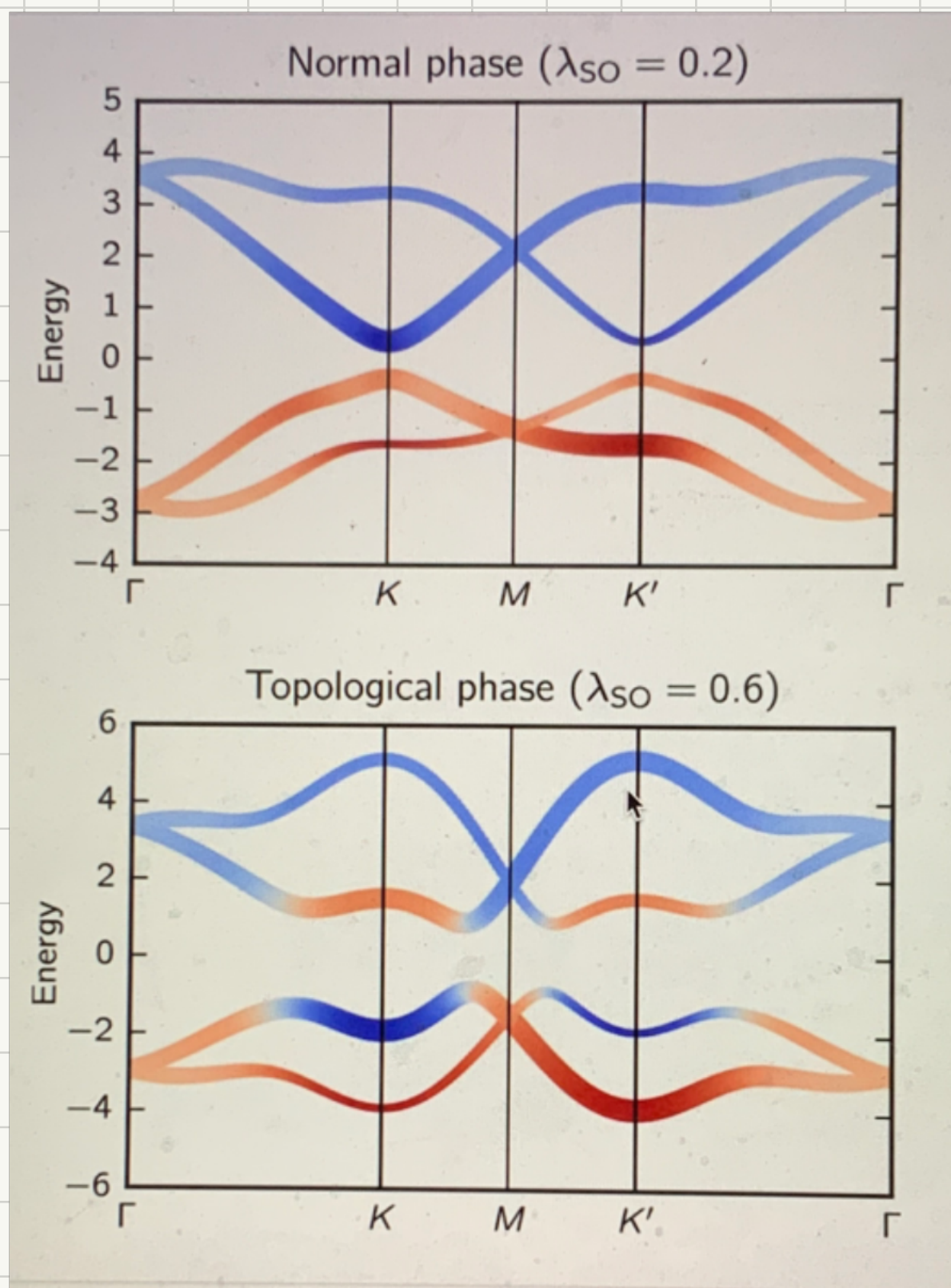
$$x = k_x \frac{a}{2}$$

$$y = k_y \frac{\sqrt{3}}{2} a$$

band
structure

identical band
structure near

$$K \leftrightarrow K'$$



6.4 Topological effect in Kane-Mele model: Quantum Spin Hall effect

Let us first consider a special case w/o Rashba

$$\lambda_R = 0$$

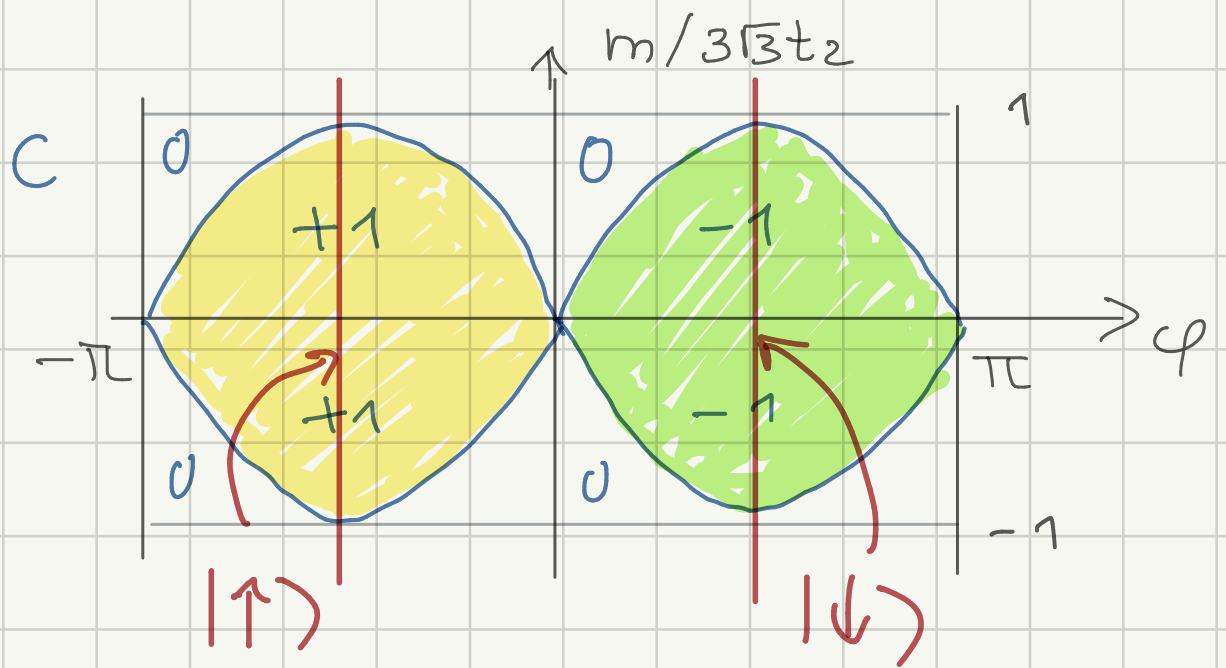
$\Rightarrow$ Spin degrees decouple!

$\Rightarrow$ We have two copies of the Haldane model with

$$\phi = \pm \frac{\pi}{2} \quad \text{for } \uparrow \text{ and } \downarrow$$

as $S_z = \pm 1$ in term with λ_{SO}

Haldane phase diagram



$$\lambda_{SO}|_{k\pi} = -3\sqrt{3}t_2 \sin \phi|_{\pi} = \pm 3\sqrt{3}t_2|_{\pi}$$

$$\lambda_I|_{k\pi} = m|_{\pi}$$

$\Rightarrow$ Chern number for spin up and down

$$(303) \quad Ch_{\uparrow} = \begin{cases} +1 & 3\sqrt{3}\lambda_{so} > \lambda_I \\ 0 & -\lambda_I \leq 3\sqrt{3}\lambda_{so} \leq \lambda_I \\ -1 & 3\sqrt{3}\lambda_{so} < -\lambda_I \end{cases}$$

$$(304) \quad Ch_{\downarrow} = \begin{cases} -1 & 3\sqrt{3}\lambda_{so} > \lambda_I \\ 0 & -\lambda_I \leq 3\sqrt{3}\lambda_{so} \leq \lambda_I \\ +1 & 3\sqrt{3}\lambda_{so} < -\lambda_I \end{cases}$$

As expected since the KM model is TR invariant the total Chern number vanishes in all regions

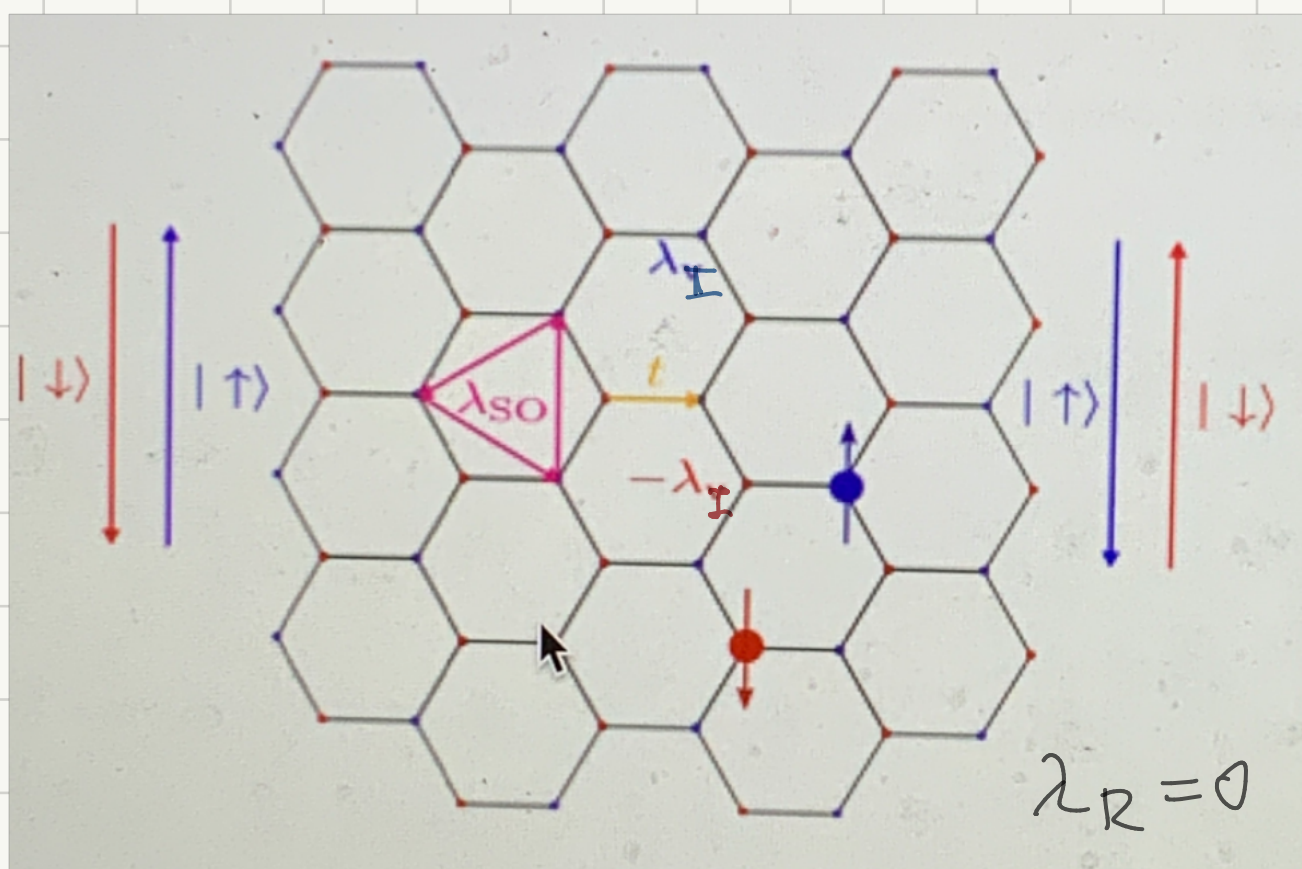
$$(305) \quad Ch = Ch_{\uparrow} + Ch_{\downarrow} = 0$$

The quantization of $Ch_{\uparrow} = -Ch_{\downarrow}$ in the topologically nontrivial phase $|\lambda_{so}| > \lambda_I$ leads to protected helical edge modes and a quantized spin Hall conductivity

$$(307) \quad \sigma_{xy}^{\uparrow} = -\sigma_{xy}^{\downarrow} = \pm \frac{e^2}{h}$$

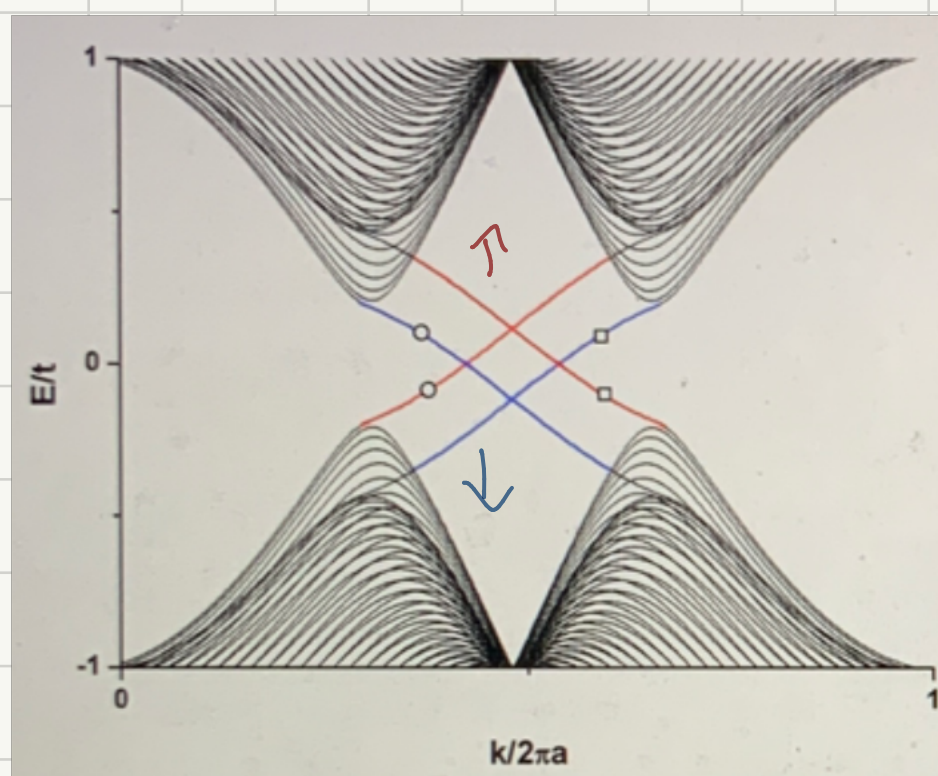
Quantum Spin Hall effect

helical edge currents

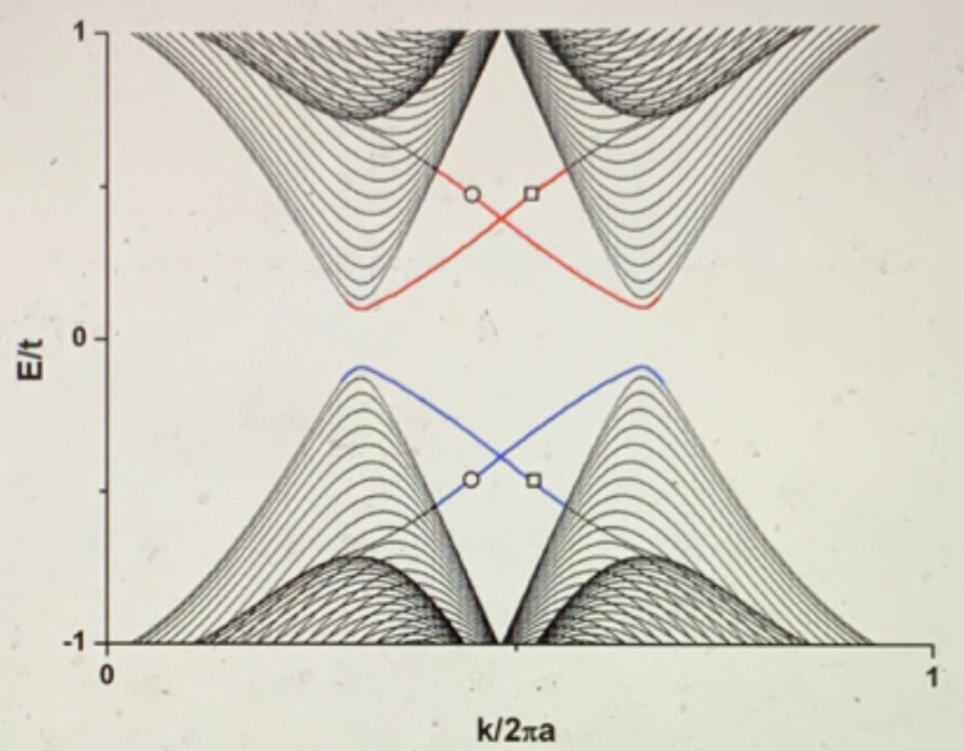


two cases?

$|\uparrow\rangle \downarrow \uparrow |\downarrow\rangle$
 or
 $|\downarrow\rangle \downarrow \uparrow |\uparrow\rangle$



$$\lambda_{SO} = 0.06 \quad \lambda_I = 0.12 \\ t = 1$$

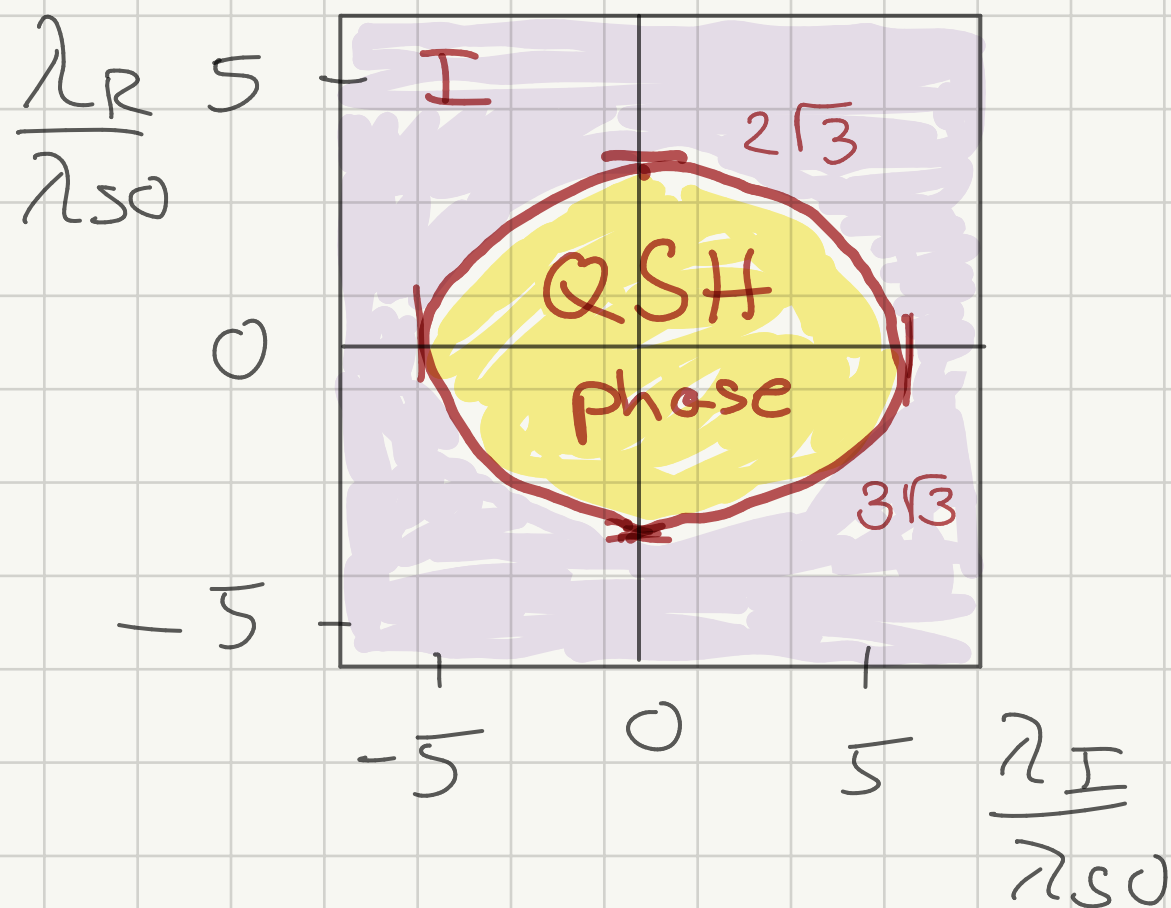


$$\lambda_{SO} = 0.06 \quad \lambda_I = 0.4 \\ t = 1$$

Now we can extend the discussion to a non-vanishing Rashba spin-orbit coupling

$$\lambda_R \neq 0$$

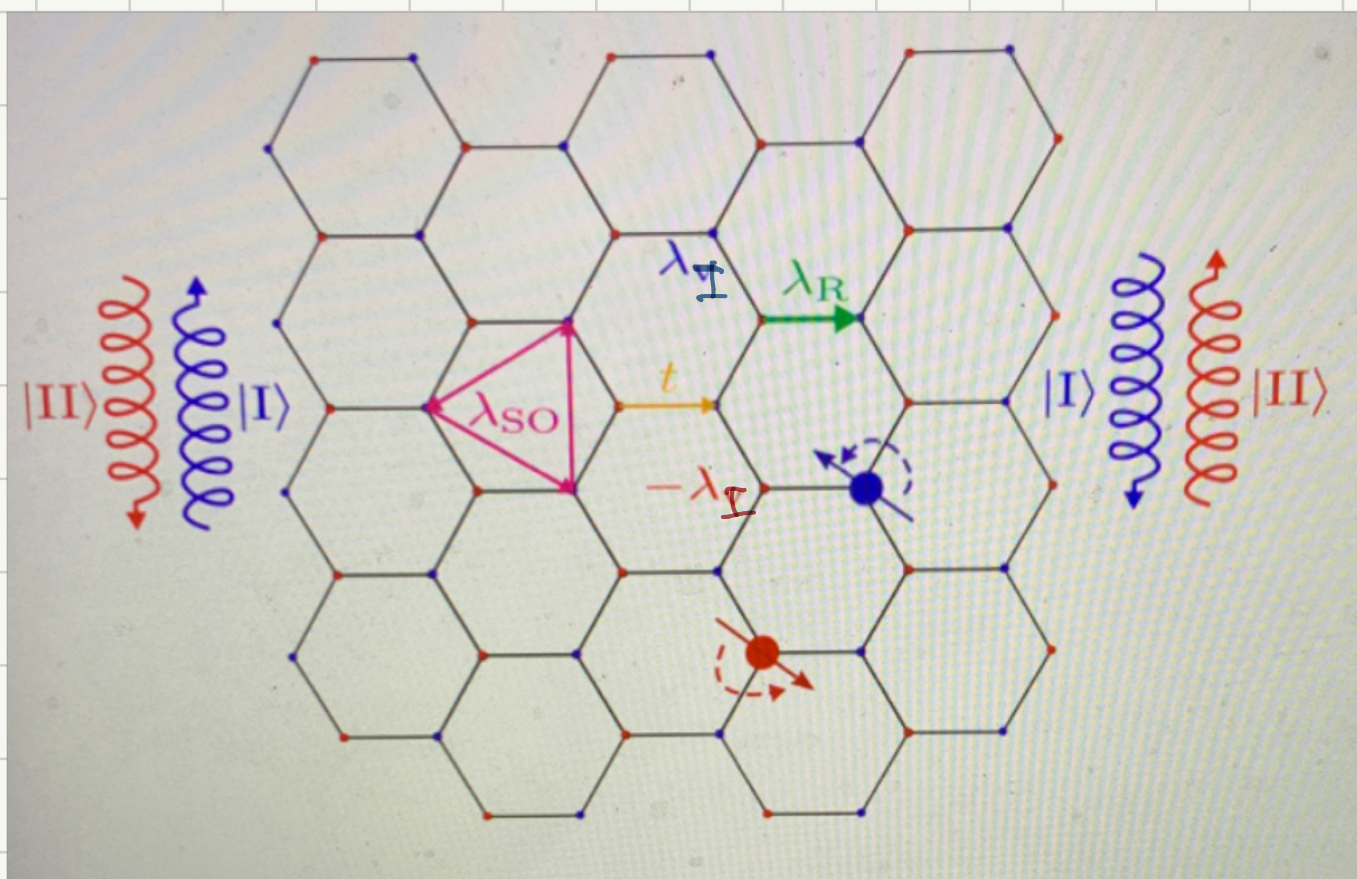
Phase with edge modes extends to finite Rashba
Spin-orbit coupling



$$3\sqrt{3} \approx 5.196$$

$$2\sqrt{3} \approx 3.464$$

With SOC edge modes rotate spin!



two cases
from above
cannot be
distinguished
anymore

The existence of robust helical edge modes is
protected by the band gap and TR Symmetry

symmetry-protected topology

What is the topological invariant?

for $\lambda_D = 0$

$$\nu_2 \equiv \frac{1}{2} |Ch_{\uparrow} - Ch_{\downarrow}| \quad (308)$$

but what for $\lambda_D \neq 0$?

7. $\mathbb{Z}_2$ topological invariant for TR symmetric bandstructures

7.1 Kramers doublet

For a many body (lattice) Hamiltonian with TR invariance

$$(309) \quad [\hat{T}, \hat{H}] = 0$$

$\Rightarrow$ common eigenbasis

$$|u(\vec{b})\rangle \quad \text{and} \quad \hat{T} |u(\vec{b})\rangle$$

are eigenstates with the same energy

$$(310) \quad |u_{\text{II}}(-\vec{b})\rangle = e^{i\chi(\vec{b})} \hat{T} |u_{\text{I}}(\vec{b})\rangle$$