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 Rice-Mele model for

Spin up ↑ and spin ↓ with 4×4 momentum Hamiltonian

(279)

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

Now choose

(280)

$$\Delta_\uparrow(t) = -\Delta_\downarrow(t) = \Delta \sin(t/T)$$

$$t_{1,2}(t) = t_0\left(1 \pm \varepsilon \cos(t/T)\right)$$

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

$$T = i\underline{\underline{\sigma_y}} K$$

(281)

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

$$\begin{bmatrix} 0 & -\mathbb{1}_{2\times2} \\ \mathbb{1}_{2\times2} & 0 \end{bmatrix} \begin{bmatrix} h_\uparrow^*(-k,-t) & 0 \\ 0 & h_\downarrow^*(-k,-t) \end{bmatrix} \begin{bmatrix} 0 & -\mathbb{1}_{2\times2} \\ \mathbb{1}_{2\times2} & 0 \end{bmatrix}$$

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

For this we note

$$\begin{aligned} h_\uparrow(k,t) &= \Delta_\uparrow \sigma_z - (t_1 + t_2 \cos k)\sigma_x - t_2 \sin k \, \sigma_y \\ h_\downarrow(k,t) &= \Delta_\downarrow \sigma_z - (t_1 + t_2 \cos k)\sigma_x - t_2 \sin k \, \sigma_y \end{aligned} \tag{283}$$

$$\begin{aligned} \Delta_{\uparrow,\downarrow}(-t) &= -\Delta_{\uparrow,\downarrow}(t) \\ t_{1,2}(-t) &= t_{1,2}(t) \end{aligned} \tag{284}$$

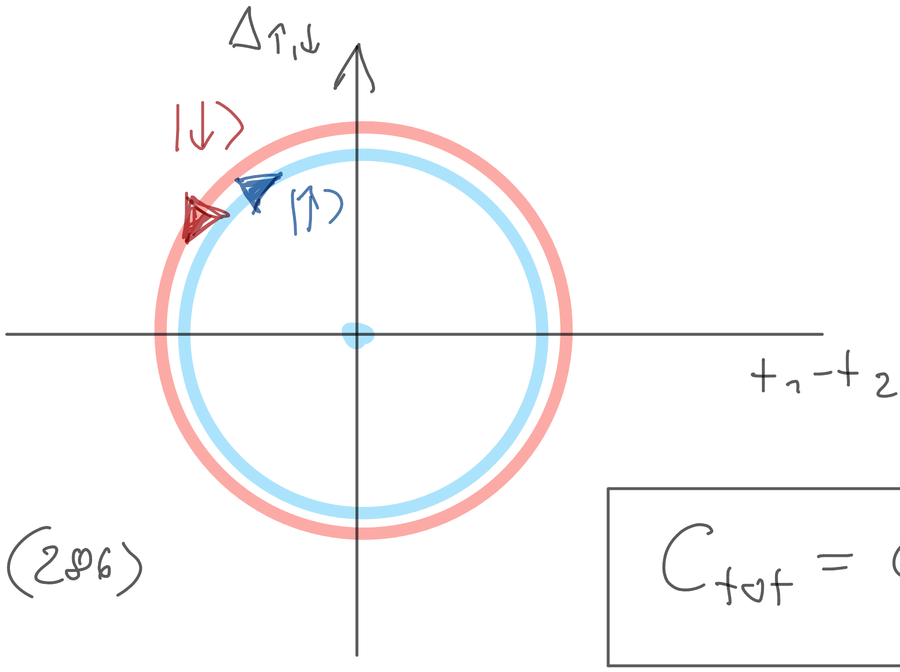
so

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

and

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

$\Rightarrow$ TR symmetry!



(286)

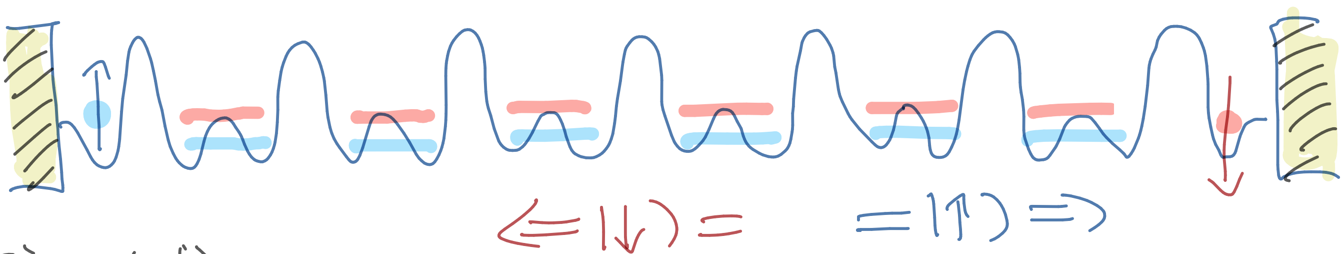
$C_\uparrow = +1$

$C_\downarrow = -1$

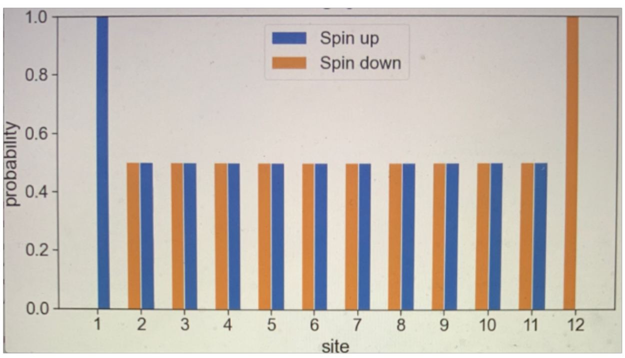
$$\boxed{C_{tot} = C_\uparrow + C_\downarrow = 0}$$

as expected from TR symmetry

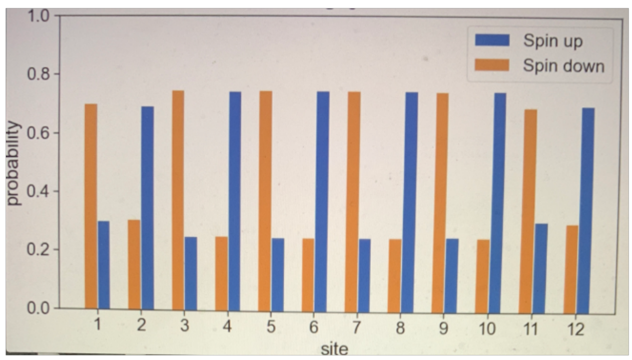
No net transport of charge, but spin pump

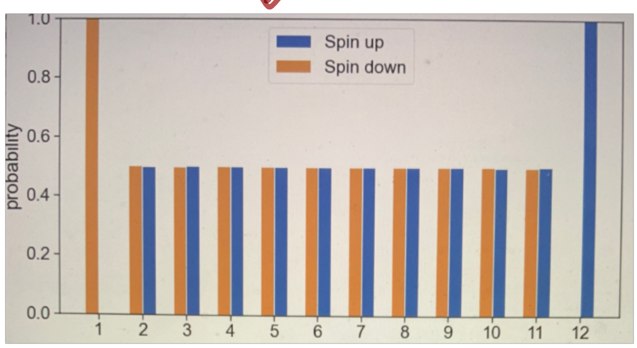


Simulation



$t = 0$





$t = T$

There is a topological quantum number

$$\boxed{\nu_2 = \frac{1}{2}\left|C_\uparrow - C_\downarrow\right|} \tag{287}$$

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

This model is however oversimplified 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.

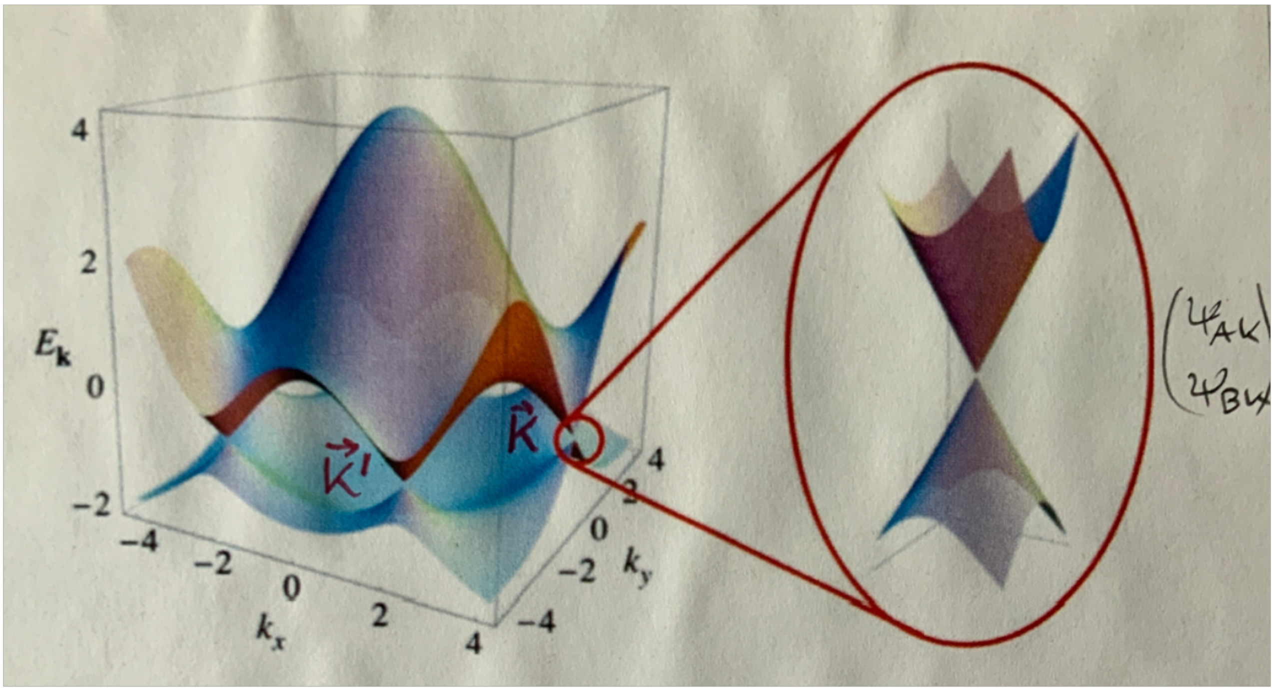
6.2 Continuum version of Kane-Mele model

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)

$$\underline{h}(\vec{K}+\delta\vec{k}) = -\frac{3}{2}t_1\left(\delta k_x \underline{\sigma}_x + \delta k_y \underline{\sigma}_y\right) \tag{288}$$
$$\underline{h}(\vec{K}'+\delta\vec{k}) = -\frac{3}{2}t_1\left(-\delta k_x \underline{\sigma}_x + \delta k_y \underline{\sigma}_y\right)$$

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) $$\hat{\underline{\psi}} = \left(\hat{\psi}_{AK}, \hat{\psi}_{BK}, \hat{\psi}_{AK'}, \hat{\psi}_{BK'}\right)$$

and introduce the real-space Hamiltonian

(290) $$\boxed{H_0 = -i\hbar v_F\, \hat{\underline{\psi}}^{\dagger}(\bar{r})\left[\sigma_x \tau_z \partial_x + \sigma_y \partial_y\right] \hat{\underline{\psi}}(\bar{r})}$$

- σ_x, σ_y Pauli matrices in (ψ_{AK}, ψ_{BK}) and $(\psi_{AK'}, \psi_{BK'})$
- $$\tau_z = \begin{pmatrix} \mathbb{1}_2 & 0 \\ 0 & -\mathbb{1}_2 \end{pmatrix} \begin{array}{l} \leftarrow K \\ \leftarrow K' \end{array}$$

$$v_F = -\frac{3}{2} a t,$$

in matrix form

(291)
$$H_0 = -i\hbar v_F \underline{\vec{\psi}}^+ \begin{bmatrix} \sigma_x \partial_x + \sigma_y \partial_y & 0 \\ 0 & -\sigma_x \partial_x + \sigma_y \partial_y \end{bmatrix} \underline{\vec{\psi}}$$

Now lets add electron spin

$\underline{\psi} \to$ 8 components

and spin-orbit coupling

(292)
$$\boxed{H_{so} = \lambda_{so} \underline{\vec{\psi}}^+ \sigma_z \tau_z S_z \underline{\vec{\psi}}}$$

A, B space   K, K' space   Spin

remarks:
- H_{so} conserves TR symmetry
- H_{so} is only allowed generalization to preserve inversion $z \leftrightarrow -z$
- H_{so} opens a gap

$\Longrightarrow$ insulator!

Kane-Mele model (continuum)

(293)
$$\boxed{\begin{aligned} H = &-i\hbar v_F \underline{\vec{\psi}}^+ (\sigma_x \tau_z \partial_x + \sigma_y \partial_y) \underline{\vec{\psi}} \\ &+ \lambda_{so} \underline{\vec{\psi}}^+ S_z \sigma_z \tau_z \underline{\vec{\psi}} \end{aligned}}$$

6.3 Kane Mele model on a lattice

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

(294)
$$\boxed{H = t_1 \sum_{\langle i,j\rangle,\sigma} \hat{c}^{\dagger}_{i\sigma}\hat{c}_{j\sigma} + i\lambda_{SO}\sum_{\langle\langle ij\rangle\rangle,\sigma,\sigma'} \nu_{ij}\,\hat{c}^{\dagger}_{i\sigma}\, S^{z}_{\sigma\sigma'}\,\hat{c}_{j\sigma'}}$$

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

$$\langle ij\rangle : NN \qquad \langle\langle ij\rangle\rangle : NNN$$

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

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

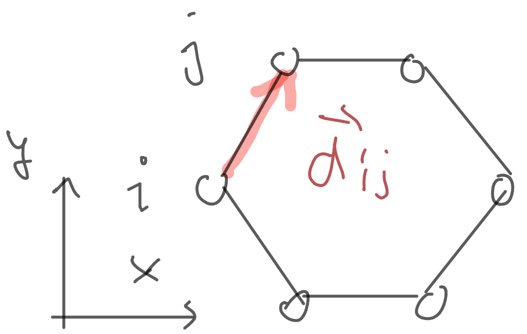
generalized spin-orbit coupling & spin mixing

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

Rashba spin-orbit coupling

$$\boxed{H_R = i\lambda_R \sum_{\langle ij\rangle} \hat{c}^{\dagger}_{i\sigma} \left[(\vec{\hat{S}} \times \vec{d}_{ij})_z \right]_{\sigma\sigma'} \hat{c}_{j\sigma'}} \tag{295}$$

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

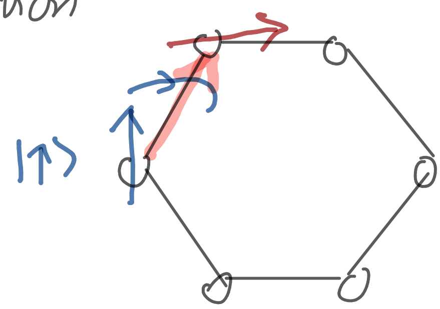


since $\vec{d}_{ij} = \alpha \vec{e}_x + \beta \vec{e}_y$

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

$\Rightarrow$ spin projection in z no longer conserved

Rashba SOC rotates the spin upon hopping of the electron



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

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

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

(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)
$$\boxed{H_I = \lambda_I \sum_{j,\sigma} \varepsilon_j \, \hat{c}^\dagger_{j\sigma} \hat{c}_{j\sigma}}$$

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

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

$$\boxed{\begin{aligned} H_{KM} = t \sum_{\langle ij\rangle} \hat{c}^\dagger_i \hat{c}_j &+ i\lambda_{SO} \sum_{\langle\langle ij\rangle\rangle} \nu_{ij} \hat{c}^\dagger_i \hat{s}^z \hat{c}_j \\ + i\lambda_R \sum_{\langle ij\rangle} \hat{c}^\dagger_i (\hat{\vec{s}} \times \vec{d}_{ij})_z \hat{c}_j &+ \lambda_I \sum_j \varepsilon_j \hat{c}^\dagger_j \hat{c}_j \end{aligned}}$$

(298) (summation over spin indices is implicit)

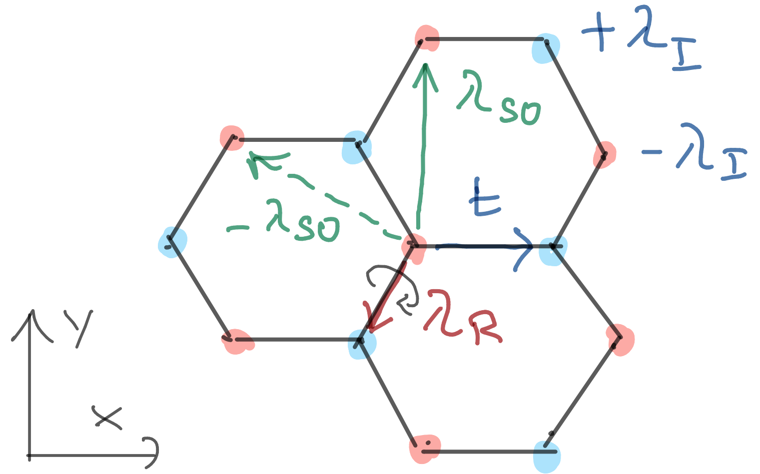
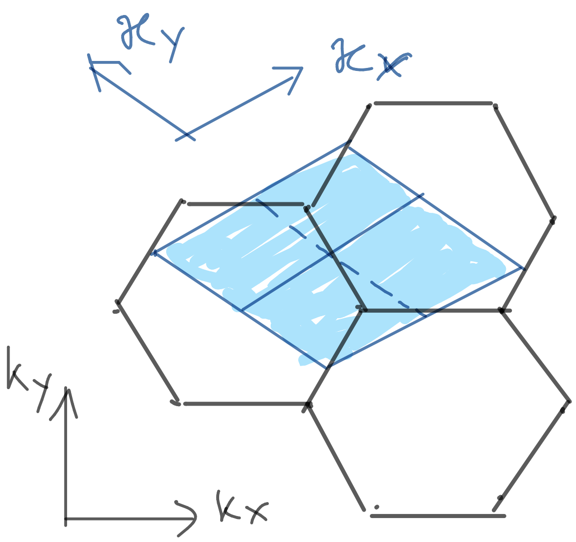


illustration of processes



Brillouin zone

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

(299) $$\boxed{H_{KM} = \sum_{\vec{k}} \underline{\tilde{c}}^{\dagger}(\vec{k})^T \, \underline{\underline{h}}_{KM}(\vec{k}) \, \underline{\hat{c}}(\vec{k})}$$

where $\underline{\hat{c}}(\vec{k}) = (\tilde{c}_{A\uparrow}, \hat{c}_{B\uparrow}, \tilde{c}_{A\downarrow}, \hat{c}_{B\downarrow})^T$

(300) $$\underline{\underline{h}}_{KM}(\vec{k}) = \begin{array}{cc} \begin{pmatrix} d_{so\uparrow} & d_t & 0 & \bar{d}_R \\ d_t^* & -d_{so\uparrow} & d_R & 0 \\ 0 & d_R^* & d_{so\downarrow} & d_t \\ \bar{d}_R^* & 0 & d_t^* & -d_{so\downarrow} \end{pmatrix} & \begin{array}{l} \left.\begin{array}{l} \\ \\ \end{array}\right\} |\uparrow\rangle \\ \left.\begin{array}{l} \\ \\ \end{array}\right\} |\downarrow\rangle \end{array} \end{array}$$

where

(301)
$$d_{so\uparrow,\downarrow} = \lambda_I \pm d_{15}$$
$$d_t = d_1 + i d_{12}$$
$$\bar{d}_R = -(d_4 + d_{23}) - i(d_3 - d_{24})$$
$$d_R = (d_4 - d_{23}) + i(d_3 + d_{24})$$

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

$$d_1 = t(1 + 2\cos x \cos y)$$

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

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

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

(3.82)

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

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

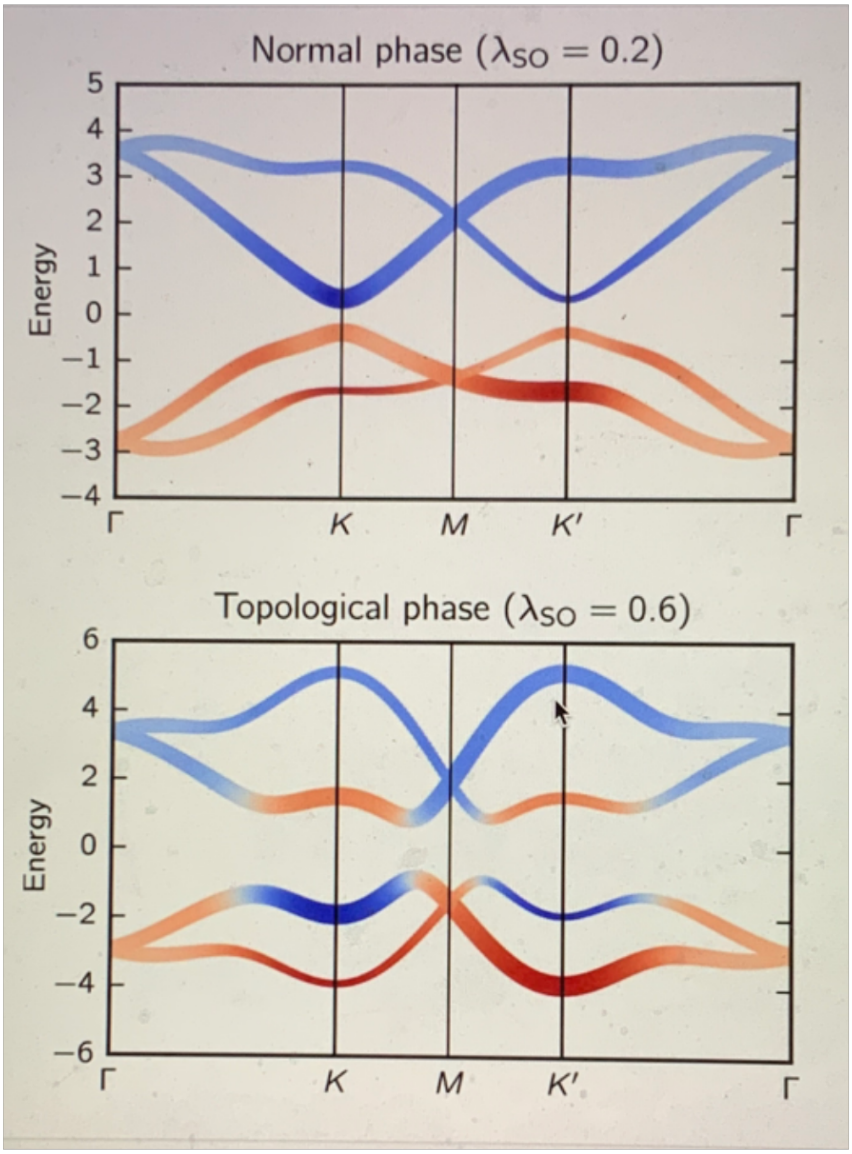
$$d_{24} = \sqrt{3}\lambda_R \sin x \cos y$$

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

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

band structure

identical band structure near $K \Leftrightarrow K'$



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

Let us first consider a special case w/o Rashba

$$\boxed{\lambda_R = 0}$$

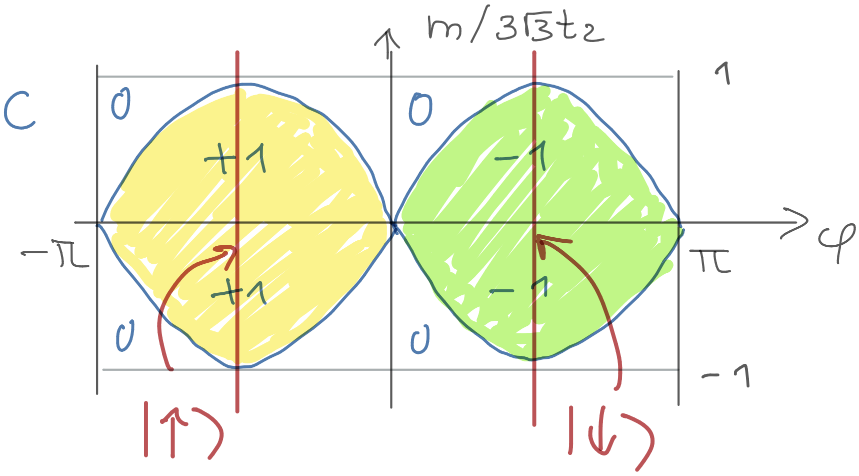
$\Rightarrow$ spin degrees decouple!

$\Rightarrow$ 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



$$\lambda_{SO}\Big|_{KM} = -t_2 \sin\phi\Big|_H = \pm t_2\Big|_H$$

$$\lambda_I\Big|_{KM} = m\Big|_H$$

$\Rightarrow$ Chern number for spin up and down

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

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

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

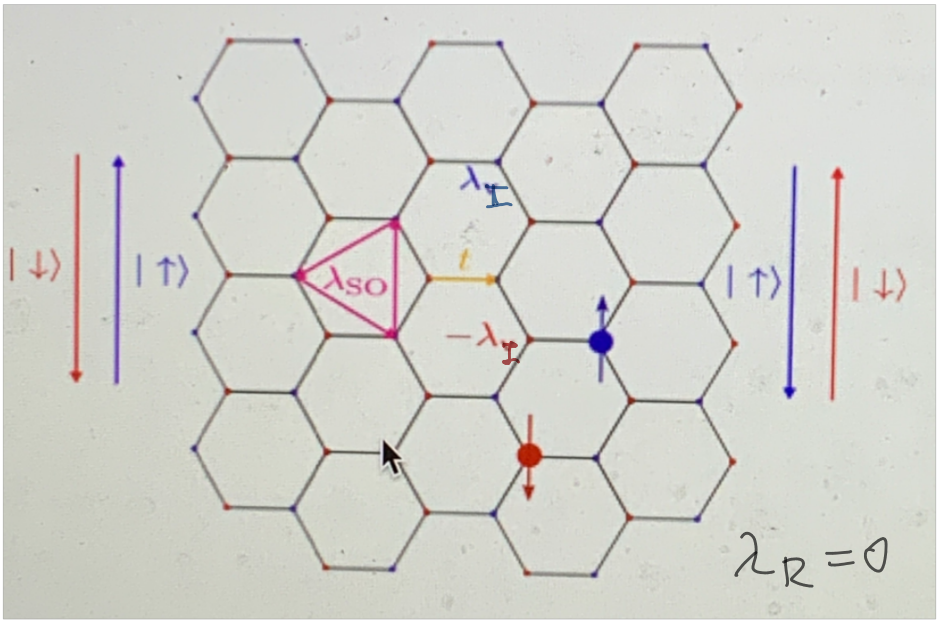
(305) $$\boxed{Ch = Ch_{\uparrow} + Ch_{\downarrow} = 0}$$

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

Quantum Spin Hall effect

helical edge currents

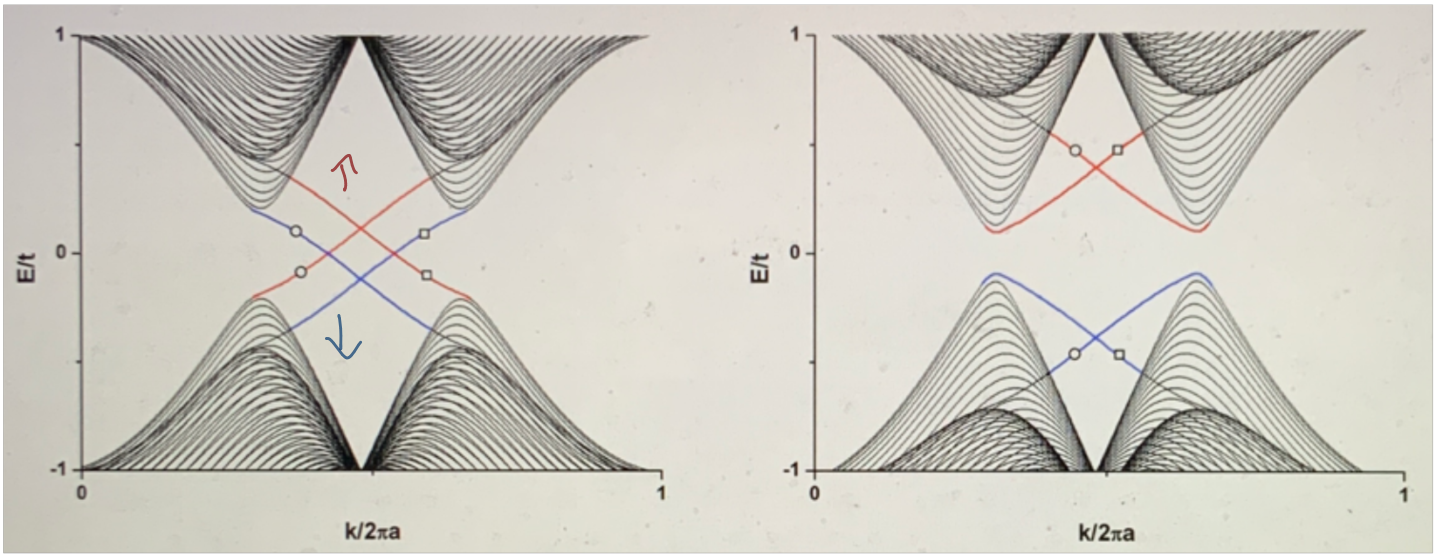


two cases?

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

or

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



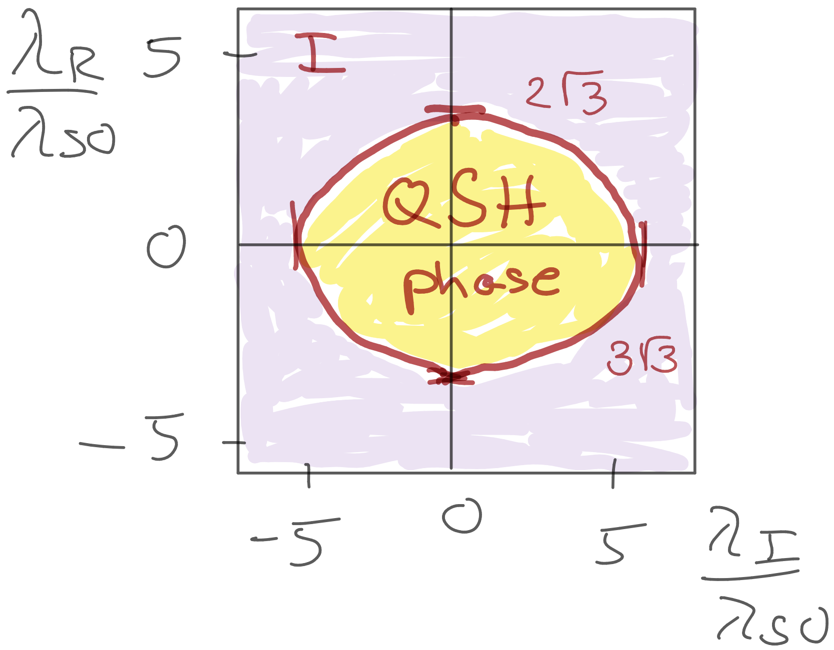
$\lambda_{SO} = 0.06 \quad \lambda_I = 0.12$
$t = 1$

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

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

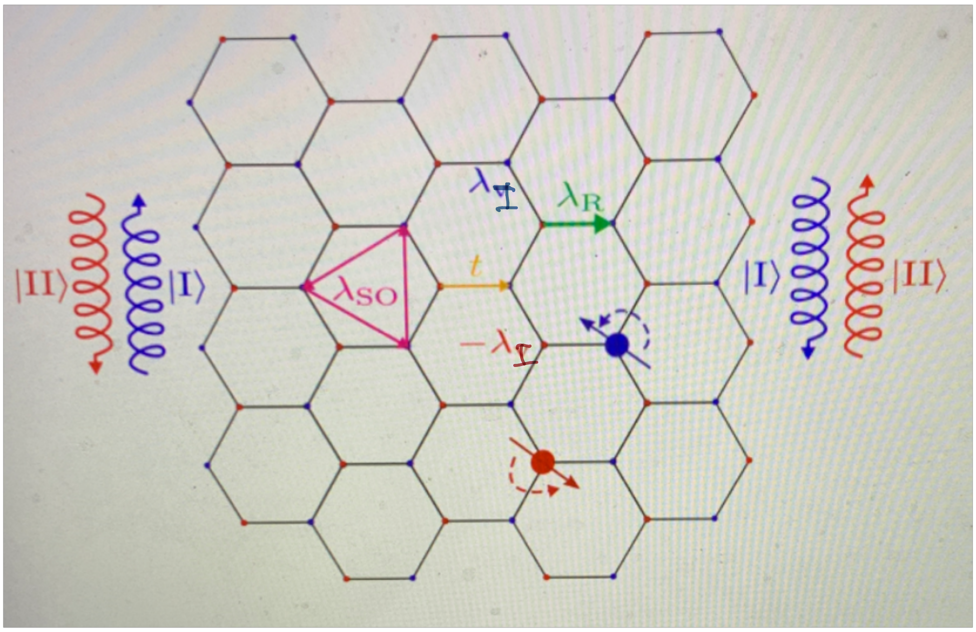
$$\boxed{\lambda_R \neq 0}$$

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



$3\sqrt{3} \simeq 5{,}196$
$2\sqrt{3} \simeq 3{,}464$

with SOC edge modes rotate spin!



two cases from above cannot be distinguished anymore

$$\boxed{\text{The existence of robust helical edge modes is protected by the band gap and TR symmetry}}$$

symmetry-protected topology

What is the topological invariant ?

for $\lambda_R = 0$ $$\boxed{\nu_2 \equiv \frac{1}{2}\left| Ch_\uparrow - Ch_\downarrow \right|} \quad (308)$$

but what for $\lambda_R \neq 0$?

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

7.1 Kramers doublett

For a many body (lattice) Hamiltonian with TR invariance

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

$\Rightarrow$ common eigenbasis

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

are eigenstates with the same energy

$$\boxed{|u_{II}(-\vec{k})\rangle = e^{i\chi(\vec{k})}\,\hat{T}\,|u_I(\vec{k})\rangle} \quad (310)$$