7. TR invariant topological bandstructures: Quantum Spin Hall Effect (QSHE) and Topological insulators (TI)

15 years after Haldane's model Kane and Mele realized that topologically non-trivial insulators exist where TR symmetry is not broken.

C.L. Kane, E.J. Mele PRL 95, 226801 (2005)

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

The Kane-Mele model arizes from a doubling of the Haldane model including a spin degree of freedom and spin-orbit coupling.

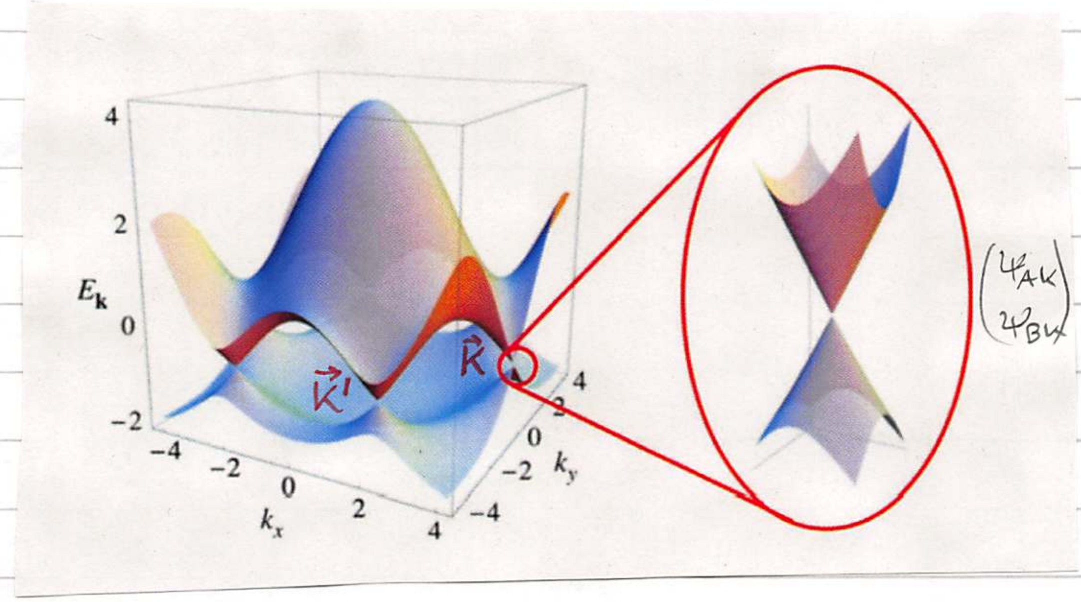
7.1 continuum version of Kane-Mele model

Let us start with the conceptually simpler continuum version of the model arizing from the low-energy limit of Graphene eq. (219)

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

(258)

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



We now introduce an effective model that treats the Dirac fermions at the $\vec{K}$ and $\vec{K}'$ points as independent species and define a 4-component state vector

$$(259) \quad \underline{\hat{\psi}}(\vec{r}) \equiv \left(\psi_{AK}(\vec{r}), \psi_{BK}(\vec{r}), \psi_{AK'}(\vec{r}), \psi_{BK'}(\vec{r})\right)^T$$

with real-space Hamiltonian

$$(260) \quad \boxed{H_0 = -i\hbar v_F \, \underline{\hat{\psi}}^{\dagger}(\vec{r}) \left(\sigma_x \tau_z \partial_x + \sigma_y \partial_y\right) \underline{\hat{\psi}}(\vec{r})}$$

σ_x, σ_y – Pauli matrices in (ψ_{AK}, ψ_{BK}) and $(\psi_{AK'}, \psi_{BK'})$ sub-spaces

$$\tau_z = \begin{pmatrix} \mathbb{1}_2 & 0 \\ 0 & -\mathbb{1}_2 \end{pmatrix} \begin{matrix} \leftarrow K \\ \leftarrow K' \end{matrix} \qquad v_F = -\frac{3}{2} a t_1$$

in matrix form (260) reads

$$(261)\quad H_0 = -i\hbar v_F\, \underline{\hat{\Psi}}^+ \begin{bmatrix} \underline{\underline{\sigma}}_x \partial_x + \underline{\underline{\sigma}}_y \partial_y & 0 \\ 0 & -\underline{\underline{\sigma}}_x \partial_x + \underline{\underline{\sigma}}_y \partial_y \end{bmatrix} \underline{\hat{\Psi}}$$

<u>addition of electron spin</u>

so far the model has no spin degree of freedom; introducing electron spin leads to a doubling of components

$\underline{\hat{\Psi}} \rightarrow 8$ components

in addition we introduce <u>spin-orbit coupling</u>

$$(262)\quad \boxed{H_{SO} = \lambda_{SO}\, \underline{\hat{\Psi}}^+ \underset{\substack{\uparrow \\ A,B}}{\sigma_z} \underset{\substack{\uparrow \\ K,K'}}{\tau_z} \underset{\substack{\uparrow \\ \uparrow,\downarrow}}{S_z} \underline{\hat{\Psi}}}$$

S_z spin operator in internal (true) spin

<u>remarks:</u>

- H_{SO} conserves <u>TR symmetry</u>
- H_{SO} is only allowed generalization which preserves inversion symmetry at x-y plane, i.e. $z \leftrightarrow -z$
- H_{SO} opens a gap $\Rightarrow$ <u>true insulator</u>

Ich show that H_{SO} emerges naturally if we look for TR invariant Hamiltonian with a finite gap.

H_0 has Dirac points $\Rightarrow$ everything which commutes with H_0

cannot open a gap → look for ΔH that anti-commutes with H_0

(263) $$H_0(\vec{K}+\delta\vec{k}) = \underline{\hat{\Psi}}^{+}\begin{bmatrix} \underline{\underline{h}}_\uparrow(\delta\vec{k}) & 0 \\ 0 & \underline{\underline{h}}_\downarrow(\delta\vec{k}) \end{bmatrix}\underline{\hat{\Psi}}$$ only part close to $\vec{K}$

where

$$\underline{\underline{h}}_\uparrow(\delta\vec{k}) = \underline{\underline{h}}_\downarrow(\delta\vec{k}) = \delta k_x \underline{\underline{\sigma}}_x + \delta k_y \underline{\underline{\sigma}}_y$$

$$\Rightarrow \qquad \Delta H = D\,\underline{\underline{\sigma}}_z$$

D is still a matrix in the internal spin

(i) $D = m\,\mathbb{1}$ breaks I symmetry

(ii) $D = S_z$!

thus

(264) $$\Delta H(\vec{K}+\delta\vec{k}) = S_z\sigma_z = \begin{array}{cc} \begin{bmatrix} \sigma_z & 0 \\ 0 & -\sigma_z \end{bmatrix} & \begin{matrix} \uparrow \\ \downarrow \end{matrix} \end{array}$$

Now lets construct $\Delta H(\vec{K}'+\delta\vec{k})$ such that total hamiltonian is TR invariant. Since we have spinful particles

$$T = e^{-i\pi\hat{S}_y}K = -i\hat{S}_y K$$

$$T H_0(\vec{k}+\delta\vec{k})T^{-1} = \begin{bmatrix} \underline{\underline{h}}_\downarrow(\delta\vec{k})^* & 0 \\ 0 & \underline{\underline{h}}_\uparrow(\delta\vec{k})^* \end{bmatrix}$$

(265) $$= \begin{bmatrix} \delta k_x\sigma_x - \delta k_y\sigma_y & 0 \\ 0 & \delta k_x\sigma_x - \delta k_y\sigma_y \end{bmatrix} = H_0(\vec{K}'-\delta\vec{k}) = H_0(-\vec{K}-\delta\vec{k}) \checkmark$$

Now

$$T\,\Delta H(\vec{K}+\delta\vec{b})T^{-1} = -S_z\sigma_z$$

$$\underset{\uparrow}{\overset{!}{\doteq}} \quad \Delta H(-\vec{K}-\partial\vec{b}) = \Delta H(\vec{K}'-\partial\bar{b})$$

for TR invariance

$$\Rightarrow \qquad \Delta H(\vec{K}') = -S_z\sigma_z$$

This finally yields (262)

$$\underline{\underline{\Delta H = \lambda_{so}\,\hat{\underline{\psi}}^{\dagger}\sigma_z S_z \tau_z \hat{\underline{\psi}}}} \qquad \square$$

Kane-Mele model

$$H = -i\hbar v_F\,\hat{\underline{\psi}}^{\dagger}(\vec{r})\left(\sigma_x\tau_z\partial_x + \sigma_y\partial_y\right)\hat{\underline{\psi}}(r) + \lambda_{so}\,\hat{\underline{\psi}}^{\dagger}(\vec{r})\,S_z\sigma_z\tau_z\,\hat{\underline{\psi}}(r) \tag{266}$$

7.2 Kane-Mele model on a lattice

Now we want to generalize the low-energy Hamiltonian (266) to a full bandstructure model

$$H = t_1 \sum_{\langle ij\rangle,\sigma} \hat{c}^{\dagger}_{i\sigma}\hat{c}_{j\sigma} + i\lambda_{so}\sum_{\substack{\langle\langle ij\rangle\rangle\\ \sigma,\sigma'}} \nu_{ij}\,\hat{c}^{\dagger}_{i\sigma}\,S^{z}_{\sigma\sigma'}\,\hat{c}_{j\sigma'} \tag{267}$$

the first part corresponds to Graphene with isotropic hopping to nearest neighbors for both spin components

$$\langle ij \rangle \;\hat{=}\; NN \qquad \nu_{ij} = \pm 1 \quad \text{as in Haldane}$$

$$\langle\langle ij \rangle\rangle \;\hat{=}\; NNN$$

For $\varepsilon \approx 0$ (267) reduces to (266). It is possible to further generalize the Kane-Mele model by a <u>Rashba Spin-Orbit term</u>

$$\boxed{H_R = i\lambda_R \sum_{\langle ij \rangle} \hat{c}^{+}_{i\sigma} \left[\left(\vec{S} \times \vec{d}_{ij} \right)_z \right]_{\sigma\sigma'} \hat{c}_{j\sigma'}} \tag{268}$$

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

For $\varepsilon \approx 0$ H_R can be written in Fourier-space approximately

$$\begin{aligned} h_R(\vec{K} + \delta\vec{k}) &= \sigma_x S_y - \sigma_y S_x \\ h_R(\vec{K}' + \delta\vec{k}) &= -\sigma_x S_y - \sigma_y S_z \end{aligned} \tag{269}$$

H_R is TR invariant but does not open the gap. For this $\lambda_{SO} \neq 0$ is necessary.

Another possible extension which <u>breaks inversion symmetry</u> is

$$\boxed{H_I = \lambda_I \sum_{j\sigma} \varepsilon_j \, \hat{c}^{+}_{j\sigma} \hat{c}_{i\sigma}} \tag{270} \qquad \varepsilon_j = \pm 1 \text{ for A or B respectively}$$

Combining all of these elements leads to the most general form of the Kane-Mele model

$$\boxed{\begin{aligned} H_{KM} &= t_1 \sum_{\langle ij\rangle} \hat{c}_i^+ \hat{c}_j + i\lambda_{SO} \sum_{\langle\langle ij\rangle\rangle} \nu_{ij}\, \hat{c}_i^+ s^z \hat{c}_j \\ &\quad + i\lambda_R \sum_{\langle ij\rangle} \hat{c}_i^+ (\vec{s}\times\vec{d}_{ij})_z \hat{c}_j + \lambda_I \sum_j \varepsilon_j \hat{c}_j^+ \hat{c}_j \end{aligned}} \tag{271}$$

(summation of spin indizes is implicit)

7.3 Spin Quantum Hall Effect

consider first minimal model

$$\lambda_R = \lambda_I = 0$$

$\Rightarrow$ spin components decouple! I.e. we have two copies of the Haldane model for $\sigma = \uparrow$ and $\sigma = \downarrow$ particles

$\boxed{\text{spin } \uparrow}$

$$\begin{aligned} \underline{\underline{h}}(\vec{K}+\delta\vec{k}) &= \delta k_x \sigma_x + \delta k_y \sigma_y + \lambda_{SO}\sigma_z \\ \underline{\underline{h}}(\vec{K}'+\delta\vec{k}) &= -\delta k_x \sigma_x + \delta k_y \sigma_y - \lambda_{SO}\sigma_z \end{aligned} \tag{272}$$

this corresponds to a (rotated) Haldane model

$$\delta k_x\big|_H \hat{=} \delta k_y \qquad \delta k_y\big|_H \hat{=} -\delta k_x$$

$$\frac{3}{2} t_1\big|_H \hat{=} -1 \qquad m\big|_H = 0$$

$$-3\sqrt{3}\, t_2 \sin\phi = \lambda_{SO}$$

Haldane was topologically non-trivial for $\phi \neq 0, \pm\pi$

(273) $$\boxed{Ch_\uparrow = \begin{cases} 1 & \lambda_{SO} > 0 \\ -1 & \lambda_{SO} < 0 \end{cases}}$$

spin ↓

(274)
$$\underline{h}(\vec{K}+\delta\vec{b}) = \delta k_x \sigma_x + \delta k_y \sigma_y - \lambda_{SO}\sigma_z$$
$$\underline{h}(\vec{K}'+\delta\vec{b}) = -\delta k_x \sigma_x + \delta k_y \sigma_y + \lambda_{SO}\sigma_z$$

corresponds again to a rotated Haldane model with

$$-3\sqrt{3}\, t_2 \sin\phi = -\lambda_{SO}$$

so

$$\boxed{Ch_\downarrow = \begin{cases} -1 & \lambda_{SO} > 0 \\ +1 & \lambda_{SO} < 0 \end{cases}}$$

The Chern number of both spin components is exactly opposite. The total Chern number vanishes.

$$Ch = Ch_\uparrow + Ch_\downarrow = 0$$

⇒ Quantum Spin-Hall Effect

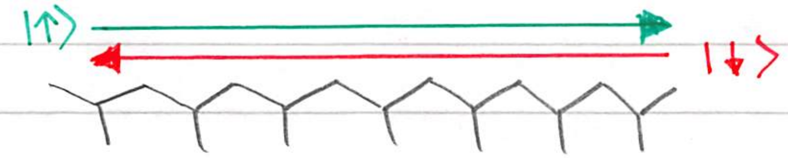
remarks:

(i) separation into ↑ and ↓ nolonger holds if there is a non-vanishing Rashba spin-orbit coupling. In this case the Chernnumber of the spin components are no good topological quantum numbers anymore!

⇒ need for a new topological quantum number!

(ii) At the edges of 2D QSH-Insulators there are pairs of edgemodes with opposite chirality

for $\lambda_R = \lambda_I = 0$ these edge modes correspond to spin-up (↑) and spin-down (↓) particles



If there is no TR-breaking impurity (magnetic impurity) there is no coupling between the two counterpropagating edge-modes (holds al. for $\lambda_R \neq 0$)

The existence of robust helical (chiral + antichiral) edge modes is protected by the band gap and TR symmetry