7. TR invariant topological band structure: Quantum Spin Hall Effect (QSH-E) 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 arises 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 arising from the low-energy limit of graphene e.g. (219)

$$\mathcal{H}_2 (\vec{k} + i\vec{\delta}) = -\frac{3}{2} t_c \left( \delta k_x \hat{\sigma}_x + \delta k_y \hat{\sigma}_y \right)$$

(258)

$$\mathcal{H}_2 (\vec{k}' + i\vec{\delta}) = -\frac{3}{2} t_c \left( -\delta k_x \hat{\sigma}_x + \delta k_y \hat{\sigma}_y \right)$$
We now introduce an effective model that treats the Dirac fermions at the $\overline{K}$ and $\overline{K}'$ points as independent species and define a 4-component state vector

$$\hat{\psi}(\mathbf{r}) = \begin{pmatrix} \psi_{AK}(\mathbf{r}) & \psi_{BK}(\mathbf{r}) & \psi_{AK'}(\mathbf{r}) & \psi_{BK'}(\mathbf{r}) \end{pmatrix}^T$$

with real-space Hamiltonian

$$H_0 = -i\hbar v_F \frac{\partial^2}{\partial\mathbf{r}^2} \left( 6x^2 \nabla_x^2 + 6y \nabla_x \nabla_y \right) \hat{\psi}(\mathbf{r})$$

$6x, 6y$ - Poincare matrices in $(2\psi_{AK}, 2\psi_{BK})$ and $(2\psi_{AK'}, 2\psi_{BK'})$ sub-spaces

\[ t_2 = \begin{pmatrix} I_2 & 0 \\ 0 & -I_2 \end{pmatrix} \leq K \quad \quad \quad v_F = -\frac{3}{2} \alpha \beta_1 \]

in matrix form (260) reads
\[ H_0 = -i\hbar \nabla \cdot \begin{pmatrix} \phi \cdot \nabla + \frac{\partial}{\partial y} & 0 \\ 0 & -\frac{\partial}{\partial x} + \frac{\partial}{\partial y} \end{pmatrix} \psi \]

**Addition of electron spin**

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

\[ \begin{pmatrix} \uparrow \\ \downarrow \end{pmatrix} \rightarrow \begin{pmatrix} \uparrow \uparrow \\ \downarrow \downarrow \end{pmatrix} \text{components} \]

In addition we introduce spin-orbit coupling.

\[ H_{so} = \lambda_{so} \begin{pmatrix} \Phi^+ & \Phi \\ \Phi & -\Phi^- \end{pmatrix} \]

\[ \begin{pmatrix} A & B & K \mu' & T \nu \\ A & B & K \mu' & T \nu \end{pmatrix} \]

\[ S_z \text{ spin operator in internal (true) spin} \]

**Remarks:**

- \( H_{so} \) conserves TR symmetry.
- \( H_{so} \) is only allowed generalization which preserves inversion symmetry at x-y plane, i.e., \( z \leftrightarrow -z \).
- \( H_{so} \) opens a gap \( \Rightarrow \) true insulator.

**Note:**

We show that \( H_{so} \) emerges naturally if we look for TR invariant Hamiltonian with a finite gap.

\( H_0 \) has Dirac points \( \Rightarrow \) every off which commutes with \( H_0 \).
cannot open a gap \rightarrow look for a \textit{field} that anti-commutes with $H_0$

\begin{equation}
H_0 (K + \delta \vec{b}) = \hat{\gamma}^4 \begin{bmatrix}
\delta \hat{b} & 0 \\
0 & \delta \hat{b}
\end{bmatrix} \hat{\gamma}^4 \text{ only part close to } K
\end{equation}

where
\begin{align*}
\delta \hat{b}_x &= \delta \hat{b}_y = \delta k_x \hat{e}_x + \delta k_y \hat{e}_y
\end{align*}

\Rightarrow
\begin{equation}
\Delta H = D \hat{g}_2
\end{equation}

$D$ is still a matrix in the chiral spin

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

(ii) $D = S_2$

Thus
\begin{equation}
\Delta H (K + \delta \vec{b}) = S_2 \hat{g}_2 = \begin{bmatrix}
\delta \omega & 0 \\
0 & -\delta \omega
\end{bmatrix}
\end{equation}

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

\begin{equation}
T = e^{-i \vec{S}_y \cdot \vec{K}} = -i \hat{S}_y \cdot \vec{K}
\end{equation}

\begin{equation}
T H_0 (K + \delta \vec{b}) T^{-1} = \hat{\gamma}^4 \begin{bmatrix}
\delta \hat{b} \hat{b}^* & 0 \\
0 & \delta \hat{b} \hat{b}^*
\end{bmatrix} \hat{\gamma}^4 = H_0 (K' + \delta \vec{b})
\end{equation}

\begin{equation}
= \begin{bmatrix}
\delta k_x \hat{e}_x - \delta k_y \hat{e}_y & 0 \\
0 & \delta k_x \hat{e}_x - \delta k_y \hat{e}_y
\end{bmatrix} = H_0 (K' + \delta \vec{b})
\end{equation}
Now
\[ T \Delta H(\hat{k} + \delta \hat{b})T^{-1} = -S \delta_2 \]
\[ \frac{1}{\mathcal{V}} \Delta H(-\hat{k} - \delta \hat{b}) = \Delta H(\hat{k} - \delta \hat{b}) \]
for TR invariance

\[ \Rightarrow \Delta H(\hat{k}') = -S \delta_2 \]

This finally yields (262)

\[ \Delta H = \lambda_{so} \frac{\hat{z}^4}{\mathcal{V}} \delta_2 S \hat{z} \hat{z} \frac{\hat{p}^2}{\mathcal{V}} \]

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**Kane-Heine model**

(266)
\[ H = -i \hbar \gamma_4 \frac{\hat{p}^4}{\mathcal{V}}(\hat{r}) \left( \partial_x \hat{z} \partial_x + \partial_y \partial_y \right) \frac{\hat{p}^2}{\mathcal{V}}(\hat{r}) + \lambda_{so} \frac{\hat{z}^4}{\mathcal{V}}(\hat{r}) S \delta \delta_2 \hat{z} \hat{z} \frac{\hat{p}^2}{\mathcal{V}}(\hat{r}) \]

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7.2 **Kane-Heine model on a lattice**

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

(267) \[ H = t \sum_{\langle \mathbf{i}, \mathbf{j} \rangle, \mathbf{k}} \hat{c}_{\mathbf{i}\mathbf{k}}^\dagger \hat{c}_{\mathbf{j}\mathbf{k}} + i \lambda_{so} \sum_{\langle \mathbf{i}, \mathbf{j} \rangle} \mathbf{v}_{\mathbf{ij}} \hat{c}_{\mathbf{i}\mathbf{k}}^\dagger S \delta_2 \hat{c}_{\mathbf{j}\mathbf{k}} \]
the first part corresponds to Graphene with isotropic hopping to nearest neighbors for both spin components

\[ \langle \text{ij} \rangle \equiv \text{NN} \quad V_{ij} = \pm t \quad \text{on } \mu \]

\[ \langle \text{ij} \rangle \equiv \text{NNNN} \quad \text{Haldane} \]

For \( E \approx 0 \), (267) reduces to (266). It is possible to further generalize the Kane-Mele model by a Rashba spin-orbit term

\[ H_R = i \lambda \sum_{\langle \text{ij} \rangle} \mathbf{C}_i^{\dagger} \left[ (\mathbf{\epsilon} \times \mathbf{a}_{ij}) \cdot \mathbf{\sigma} \right] \mathbf{C}_j \]

where \( \mathbf{a}_{ij} \) is the vector connecting lattice sites "i" and "j".

For \( E \approx 0 \), \( H_R \) can be written in Fourier-space approximately

\[ H_R (\vec{k} + \delta \vec{k}) = - \sigma_x S_y - \sigma_y S_x \]

\[ H_R (\vec{k} + \delta \vec{k}) = - \sigma_x S_y - \sigma_y S_x \]

\( H_R \) is TR-invariant but does not open the gap. For this \( \lambda \approx 0 \) is necessary.

Another possible extension which breaks inversion symmetry is

\[ H_I = \lambda_I \sum_{j \alpha} \epsilon_j \mathbf{C}_j^{\dagger} \mathbf{C}_{j \alpha} \]

\[ \epsilon_j = \pm 1 \quad \text{for } A \text{ or } B \] respectively
Combining all of these elements leads to the most general form of the Kane-Mele model

\[
H_{km} = t_n \sum_{i,j} \tilde{c}_i^+ \tilde{c}_j + i \lambda_{so} \sum_i \tilde{e}_i \tilde{c}_i^+ \tilde{e}_j \tilde{c}_j \\
+ i \lambda_R \sum_i \tilde{c}_i^+ \left( \tilde{S}_i \times \tilde{d}_{ij} \right) \tilde{c}_j + \lambda_I \sum_j \tilde{e}_j \tilde{c}_j^+ \tilde{c}_j 
\]

(summation of spin indices is implicit)

7.3 Spin Quantum Hall Effect

Consider first minimal model

\[\lambda_R = \lambda_I = 0\]

\[\Rightarrow \text{spin components decouple! i.e. we have two copies of the Haldane model for } \sigma = 1\]
and \( \sigma = 1\) provides

\[
|\tilde{\sigma}| \Rightarrow \left( \tilde{\sigma} + \delta \tilde{B} \right) = \delta \tilde{K} \times \delta x + \delta \tilde{K} \cdot \delta y + \lambda_{so} \delta z
\]

(272)

\[
|\tilde{\sigma}'| \Rightarrow \left( \tilde{\sigma}' + \delta \tilde{B} \right) = -\delta \tilde{K}_x \delta x + \delta \tilde{K}_y \delta y - \lambda_{so} \delta z
\]

this corresponds to a (rotated) Haldane model
\[
\delta k_x |_H = \delta k_y \quad \delta k_y |_H = - \delta k_x
\]
\[
\frac{3}{2} t_2 |_H = -1 \quad m |_H = 0
\]
\[-3 \sqrt{3} t_2 \sin \phi = \lambda_{50}
\]

Haldane was topologically non-trivial for \( \phi \neq 0, \pm \pi \).

\begin{equation}
\text{Ch}^\uparrow = \begin{cases}
1 & \lambda_{50} > 0 \\
-1 & \lambda_{50} < 0
\end{cases}
\end{equation}

For spin \( \uparrow \) \:

\begin{equation}
\hbar (\vec{L} + \vec{S}) = \delta k_x \delta x + \delta k_y \delta y + \lambda_{50} \delta z
\end{equation}

\begin{equation}
\hbar (\vec{L}' + \vec{S}) = -\delta k_x \delta x + \delta k_y \delta y - \lambda_{50} \delta z
\end{equation}

corresponds again to a rotated Haldane model

with

\[-3 \sqrt{3} t_2 \sin \phi = - \lambda_{50}\]

So

\begin{equation}
\text{Ch}^\downarrow = \begin{cases}
-1 & \lambda_{50} > 0 \\
+1 & \lambda_{50} < 0
\end{cases}
\end{equation}

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

\[\text{Ch} = \text{Ch}^\uparrow + \text{Ch}^\downarrow = 0\]
Quantum Spin-Hall Effect

(i) Separation into $\uparrow$ and $\downarrow$ no longer holds if there is a non-vanishing Rashba spin-orbit coupling. In this case the Chern numbers of the spin components are no good topological quantum numbers anymore.

$\Rightarrow$ Need for a new topological quantum number

(ii) At the edges of 2D QSHI Insulators there are pairs of edge modes with opposite chirality for $\gamma_E = \gamma_f = 0$ these edge modes correspond to spin-up ($\uparrow$) and spin-down ($\downarrow$) particles

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

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