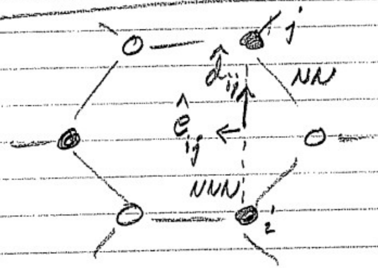
Haldane and Kane-Mele Models



$$\hat{e}_{ij} = \hat{z} \times \hat{d}_{ij}$$

Notation:

- $\sum_{ij}' = \sum_{ij}^{NN}$
- $\sum_{ij}'' = \sum_{ij}^{NNN}$
- $\nu_{ij} = \begin{cases} +1, & \hat{e}_{ij} \text{ in } \quad (ccw) \\ -1, & \hat{e}_{ij} \text{ out } \quad (cw) \end{cases}$
- $\xi_i = \pm 1$ depending on ●, ○

Haldane: (Spinless electrons!)

$$H = \Delta \sum_i \xi_i c_i^+ c_i + t \sum_{ij}' c_i^+ c_j + t_2 \sum_{ij}'' e^{i\nu_{ij}\phi} c_i^+ c_j$$

Strongest broken T at $\phi = \pi/2 \Rightarrow i t_2 \sum_{ij}'' \nu_{ij} c_i^+ c_j$

Now superpose: • Haldane for spin $\uparrow$, $\phi = \pi/2$

• Haldane for spin $\downarrow$, $\phi = -\pi/2$

$$H = \Delta \sum_i \xi_i \left(c_{i\uparrow}^\dagger c_{i\uparrow} + c_{i\downarrow}^\dagger c_{i\downarrow} \right) + \cdots$$

Herm? yes

TR? yes

$$= \Delta \sum_{i\mu} \xi_i c_{i\mu}^\dagger c_{i\mu} + t \sum_{ij}{}' \sum_\mu c_{i\mu}^\dagger c_{j\mu}$$

$$+ i t_2 \sum_{ij}{}'' \nu_{ij} \left(c_{i\uparrow}^\dagger c_{j\uparrow} - c_{i\downarrow}^\dagger c_{j\downarrow} \right)$$

Notation:

① $t_2 \to \lambda_A$

② Pauli matrices $\sigma_x, \sigma_y, \sigma_z$

Last term $= i\lambda_A \sum_{ij}{}'' \nu_{ij} \sum_{\mu\nu} \sigma_{z,\mu\nu} c_{i\mu}^\dagger c_{j\nu}$

Last term is a spin-dependent hopping, which is a kind of SOC, but it does not actually mix spin-up and spin-down sectors yet. So add one more term:

$$H = H_\Delta + H_t + H_A^{(SO)} + H_B^{(SO)}$$

$$H_\Delta = \Delta \sum_{i\mu} \xi_i \, c_{i\mu}^+ c_{i\mu}$$

$$H_t = t \sum_{ij}' \sum_{\mu} c_{i\mu}^+ c_{j\mu}$$

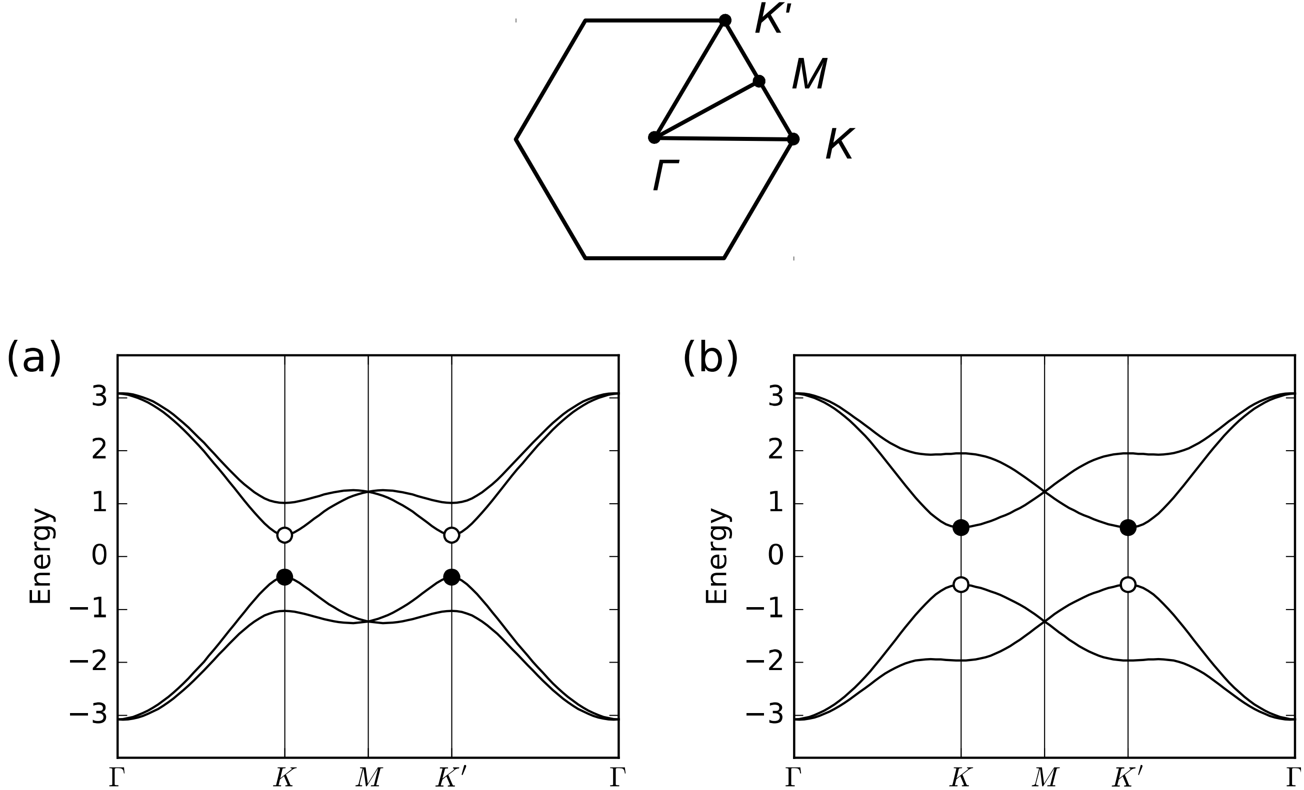
$$H_A^{(SO)} = i\lambda_A \sum_{ij}'' \nu_{ij} \sum_{\mu\nu} \hat{z} \cdot \underline{\sigma}_{\mu\nu} \, c_{i\mu}^+ c_{j\nu} \qquad (\sigma_z)$$

$$H_B^{(SO)} = i\lambda_B \sum_{ij}' \sum_{\mu\nu} \hat{e}_{ij} \cdot \underline{\sigma}_{\mu\nu} \, c_{i\mu}^+ c_{j\nu} \qquad (\sigma_x, \sigma_y)$$

$H_A^{(SO)}$ = "spin-diag SO int"

$H_B^{(SO)}$ = "spin-mixing SO int" = "Rashba int"

Note: Model has T sym! • Complex conj: $i \Rightarrow -i$
• $\sigma \Rightarrow -\sigma$



Trivial phase
Z_2=0 or ν = +

Topological phase
Z_2=1 or ν = −

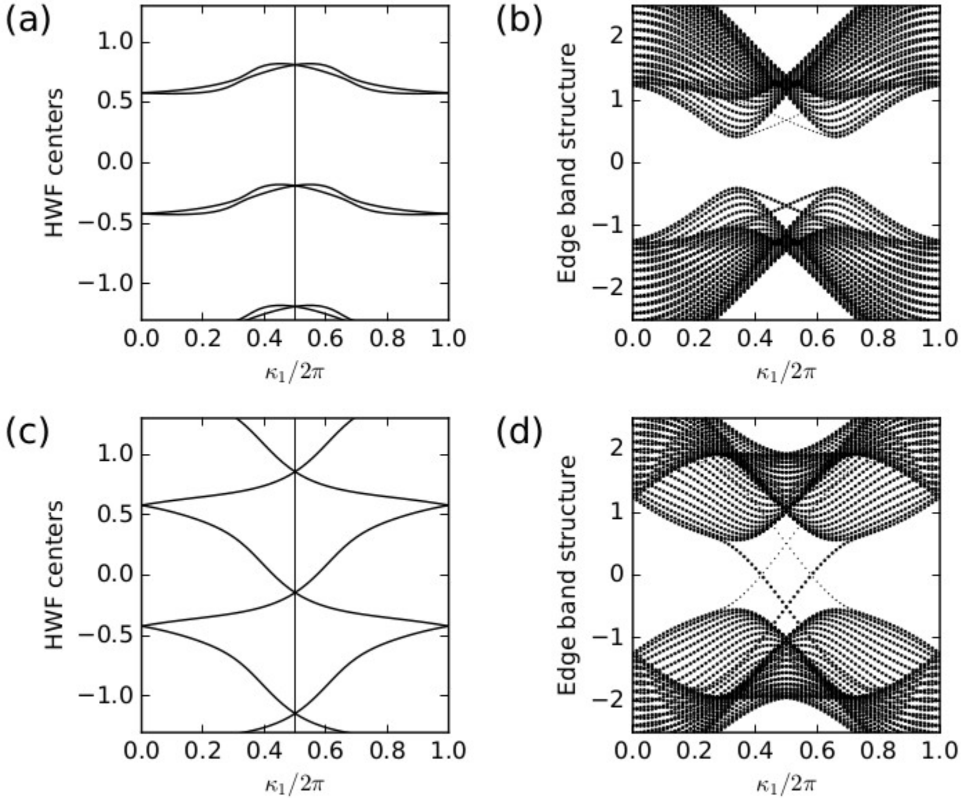


Figure 5.13 (a) Flow of hybrid Wannier centers for a Kane-Mele model in the trivial phase with $\Delta = 0.7$, $t_1 = -1.0$, $\lambda_{\mathrm{R}} = 0.05$, and $\lambda_{\mathrm{SO}} = -0.06$. (b) Edge states on a ribbon cut from the same model; those on the top and bottom edges of the ribbon are indicated by full and reduced intensity respectively. (c-d) Same as (a-b), but in the topological phase, $\lambda_{\mathrm{SO}} = -0.24$.

Quick Review: Spin-orbit

Dirac eqn, Put theo in $\frac{1}{mc^2}$ $\Rightarrow$ effective SE:

$$H = \frac{p^2}{2m} + V(r) + \underbrace{(p^4 \text{ corr} + p^6 \text{ corr} + \cdots)}_{\text{"scalar relativistic"}}$$

$$+ \frac{\hbar}{4m^2c^2}\, \underline{\sigma} \cdot (\underline{\nabla} V \times \underline{p}) + \cdots$$

$\Uparrow$ spin-orbit; $\underline{p} \to -i\hbar\underline{\nabla}$

$\to$ on p. 3 of notes: incorrectly written as $-eV$

$$\boxed{H_{SO} = \frac{\hbar}{4m^2c^2}\, \underline{\sigma} \cdot \underline{\nabla} V \times \underline{p}} \Leftarrow$$

Does not break T.

Why not? ...

$$\boxed{H_{SO}^{\text{central}} = \xi(r)\, \underline{L} \cdot \underline{S}, \quad \xi(r) = \frac{1}{2m^2c^2} \frac{1}{r} \frac{\partial V}{\partial r}}$$

3d: ~ 5 meV ?
4d: ~ 50 meV ?
5d: ~ 0.5 eV ?

SO in TB

$$H_{SO} = \frac{\hbar}{4m^2c^2}\, \boldsymbol{\sigma} \cdot \nabla V \times \mathbf{p}$$

$$= \frac{\hbar}{4mc^2}\, \boldsymbol{\sigma} \cdot \nabla V \times \mathbf{v}$$ ← probably more fundamental. frame of ref: $\nabla V = \mathcal{E} \Rightarrow B$

TB:

$$\mathbf{d}_{ij} = \mathbf{r}_j - \mathbf{r}_i$$

$$H_{ij} = \langle \varphi_i | H | \varphi_j \rangle$$ "hop from j to i" (backwards?!)

$H_{ij}\, c_i^\dagger c_j$

$$\mathbf{v}_{ij} = \langle \varphi_i | \mathbf{v} | \varphi_j \rangle$$

$$= \frac{-i}{\hbar} \langle \varphi_i | [\mathbf{r}, H] | \varphi_j \rangle$$

$$= \frac{i}{\hbar}\, \mathbf{d}_{ij} \langle \varphi_i | H | \varphi_j \rangle$$

$$\mathbf{v}_{ij} = \frac{it}{\hbar}\, \mathbf{d}_{ij} \qquad t = \langle \varphi_i | H | \varphi_j \rangle = H_{ij}.$$ need $v_{ij} = v_{ji}^*$

↑ units of hopping rate × hop dist = veloc

$$(H_{SO})_{i\mu, j\nu} = \langle \varphi_{i\mu} | H_{SO} | \varphi_{j\nu} \rangle$$

$$= \frac{\hbar}{4mc^2}\, \boldsymbol{\sigma}_{\mu\nu} \cdot (\nabla V \times \mathbf{v})_{ij}$$ ↙ mid bond

$$(H_{SO})_{i\mu,j\nu} = \langle \varphi_{i\mu} | H_{SO} | \varphi_{j\nu} \rangle$$

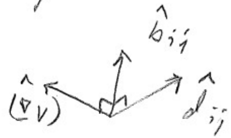
$$= \frac{\hbar}{4mc^2}\, \underline{\sigma}_{\mu\nu} \cdot (\underline{\nabla} V \times \underline{v})_{ij}$$

mid bend

↳ $\underline{\underline{\text{approx}}}$ as $\underline{\nabla} V_{mb} \times \underline{v}_{ij}$

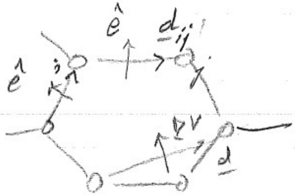
$$= \frac{i t}{4mc^2}\, \underline{\sigma}_{\mu\nu} \cdot \underline{\nabla} V_{mb} \times \underline{d}_{ij}$$

$$= i \underline{b}_{ij} \cdot \underline{\sigma}_{\mu\nu} \qquad = i\lambda\, \underline{\sigma}_{\mu\nu} \cdot \hat{b}_{ij}$$



$$\underline{b}_{ij} = \frac{t}{4mc^2}\, \underline{\nabla} V_{mb} \times \underline{d}_{ij}$$

<u>Build Kane-Mele</u>



<u>1^{st} neigh</u>

Symm: $\underline{\nabla} V_{mb} = 0$ (or $\parallel$ to $\underline{d}_{ij}$)

$\Rightarrow \underline{b}_{ij} = 0$

<u>2^{nd} neigh</u> $\quad \hat{b}_{ij} = \hat{z}$

$$\boxed{H_A^{SO} = i\lambda_A \sum_{ij}{}'' \sum_{\mu\nu} \sigma_{z,\mu\nu}\, c_{i\mu}^{\dagger} c_{j\nu}}$$

↳ $c_{i\uparrow}^{\dagger} c_{j\uparrow} - c_{i\downarrow}^{\dagger} c_{j\downarrow}$

⇑ Just 2 copies of Haldane w/ $n_{ch} = \pm 1$

But still no mixing btw. $\uparrow, \downarrow$

Add Rashba = SO due to external $\mathcal{E}_z$, or on substrate, or ...

$\nabla V_{MG} \parallel \hat{z}$

Now $\hat{b}_{ij} = \hat{z} \times \hat{d}_{ij} = \hat{e}_{ij}$!

Works for 1st or 2nd neigh; easier to put in 1st.

$$\boxed{H_B^{SO} = i \lambda_B \sum_{ij}' \sum_{\mu\nu} \hat{e}_{ij} \cdot \sigma_{\mu\nu} c_{i\mu}^{+} c_{j\nu}}$$

σ_x, σ_y off-diag mixing

$$H_{\text{Kane-Mele}} = H_\Delta + H_t + H_A^{SO} + H_B^{SO}$$

$$H = \Delta \sum_i (-)^{\tau_i} c_i^\dagger c_i + t_1 \sum_{\langle ij \rangle} (c_i^\dagger c_j + \text{h.c.}) + \lambda_{\text{SO}} \sum_{\langle\langle ij \rangle\rangle} (i c_i^\dagger \sigma_z c_j + \text{h.c.})$$
$$+ \lambda_{\text{R}} \sum_{\langle ij \rangle} (i c_i^\dagger \hat{\mathbf{e}}_{\langle ij \rangle} \cdot \boldsymbol{\sigma} c_j + \text{h.c.}) \tag{5.17}$$