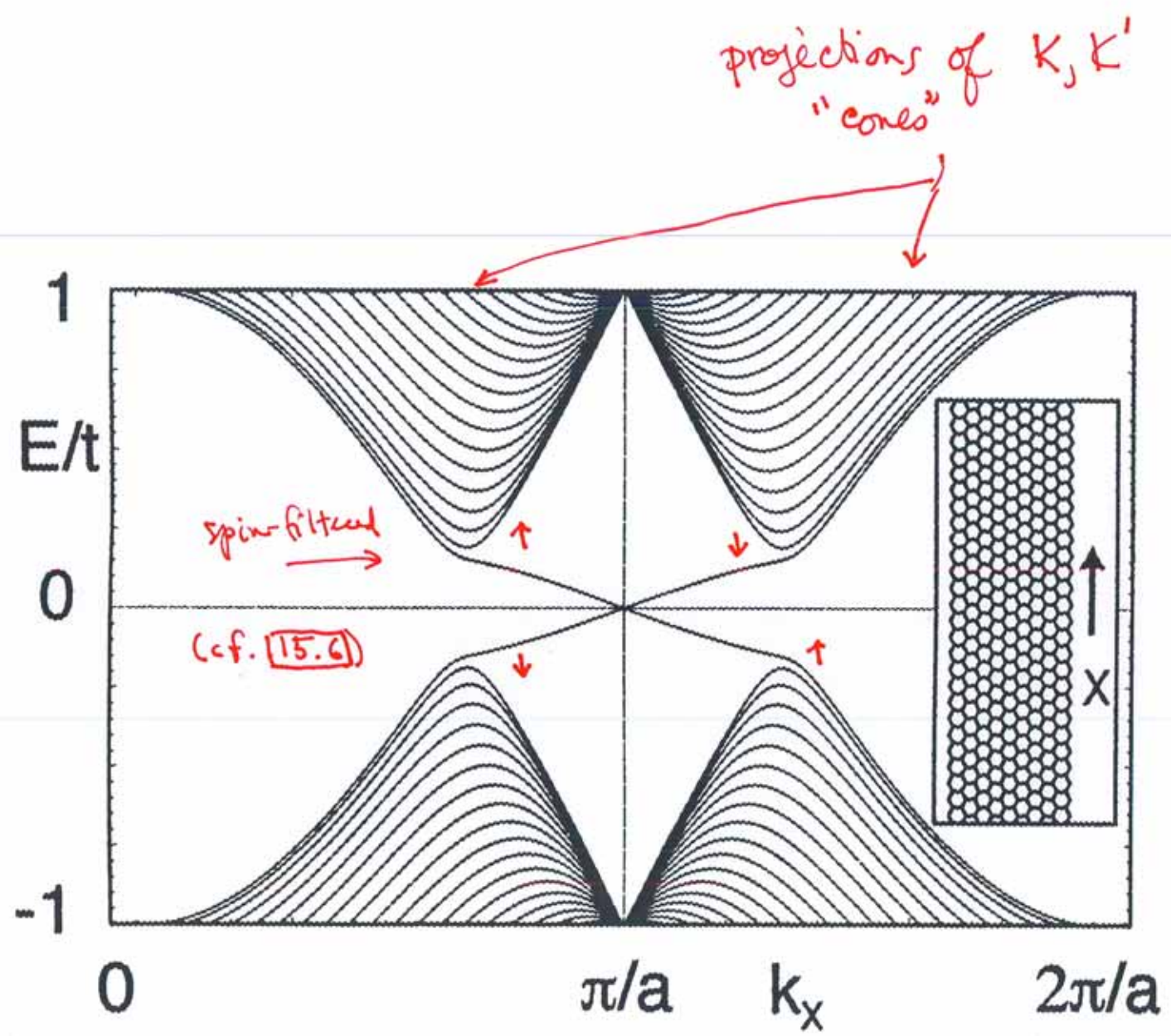
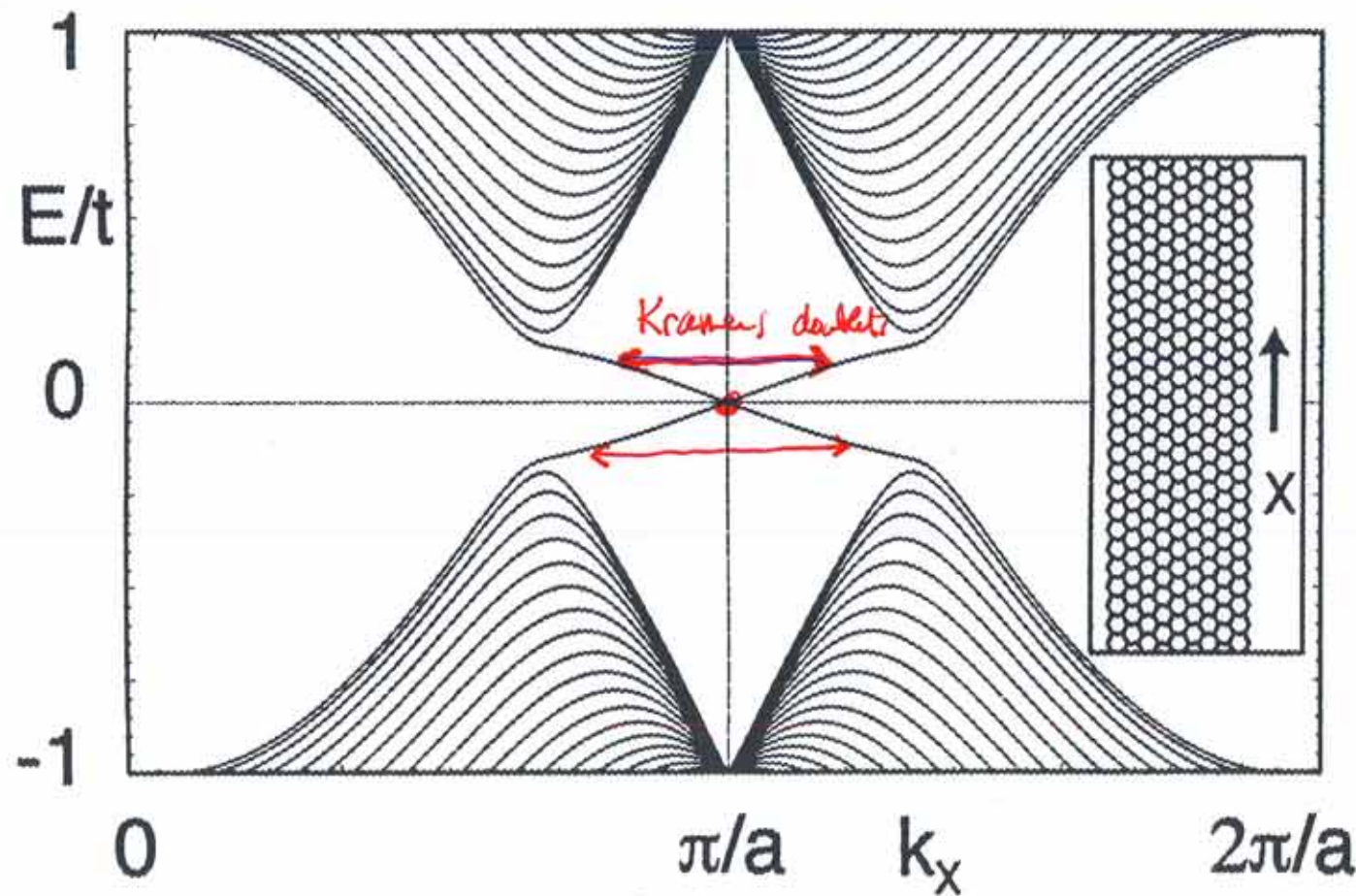


Scholium on the figures ...

(Dirac: "I understand ~~and~~ an equation when I can anticipate the properties of its solution without actually solving it.")



note: i)  $K_y$  discretized  
ii) gap opened by  $\Delta_{SO}$

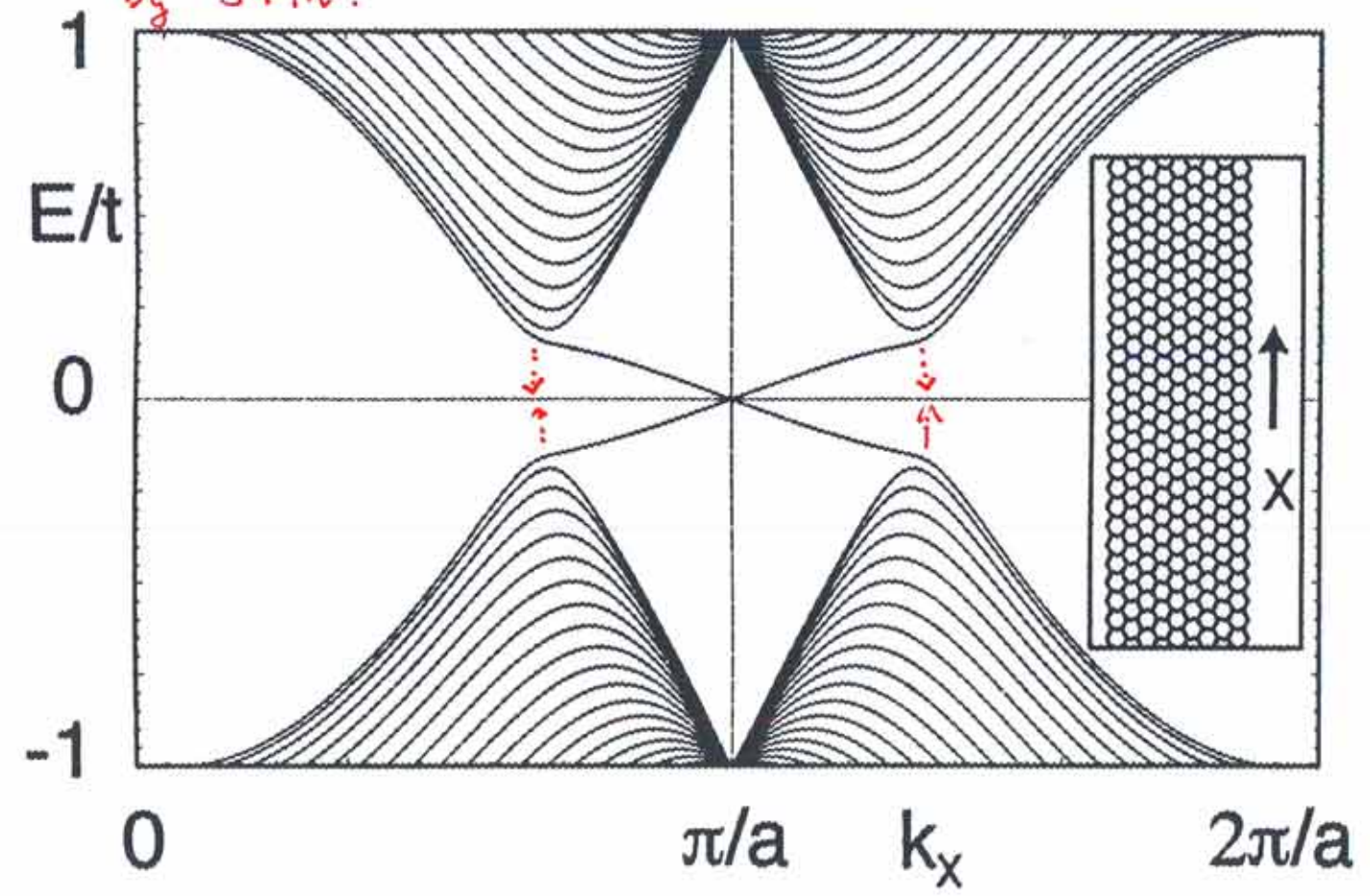


- At  $\pi/a$  ( $= -\pi/a$ ) the doublet is a crossing.
- The crossing cannot be lifted by T-invariant perturbations

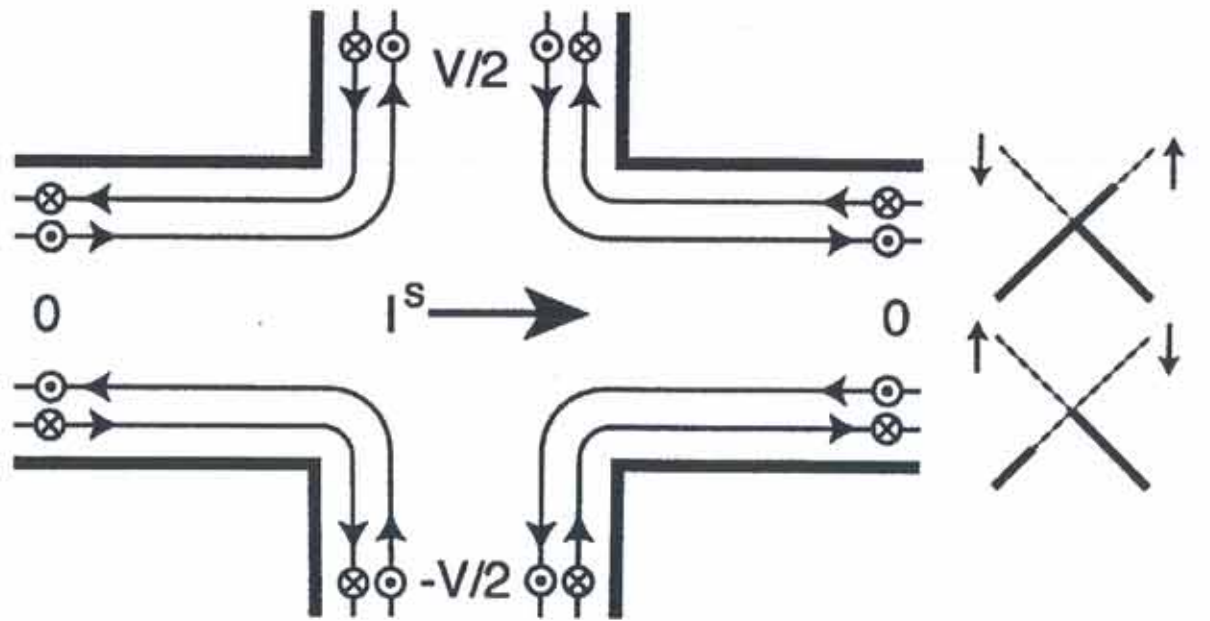
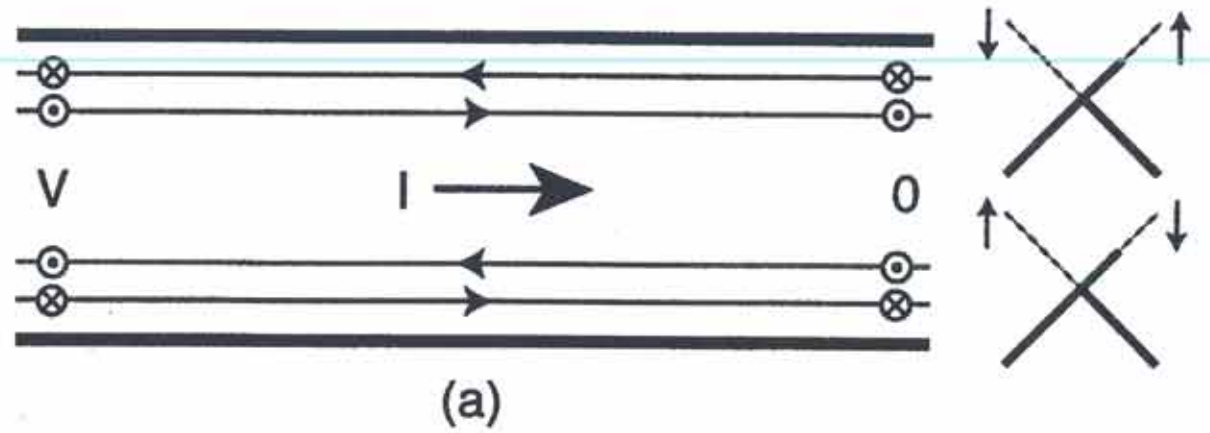


As  $\Delta_{so} \rightarrow 0$  the cones come down and the 0-modes become exactly flat.

This enhanced density of states has been observed by STM.

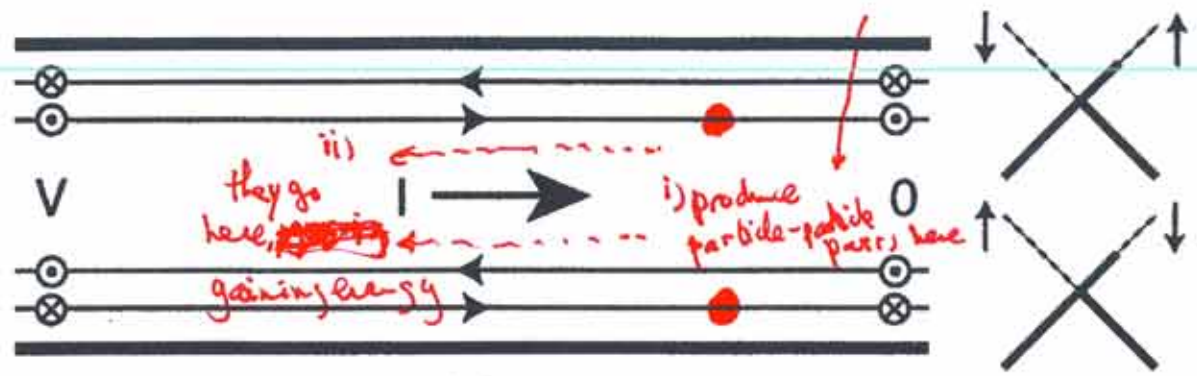


The spin-up ( $\odot$ ) <sup>current</sup> wants the wall to its left.  
The spin-down ( $\otimes$ ) current wants the wall to its right.

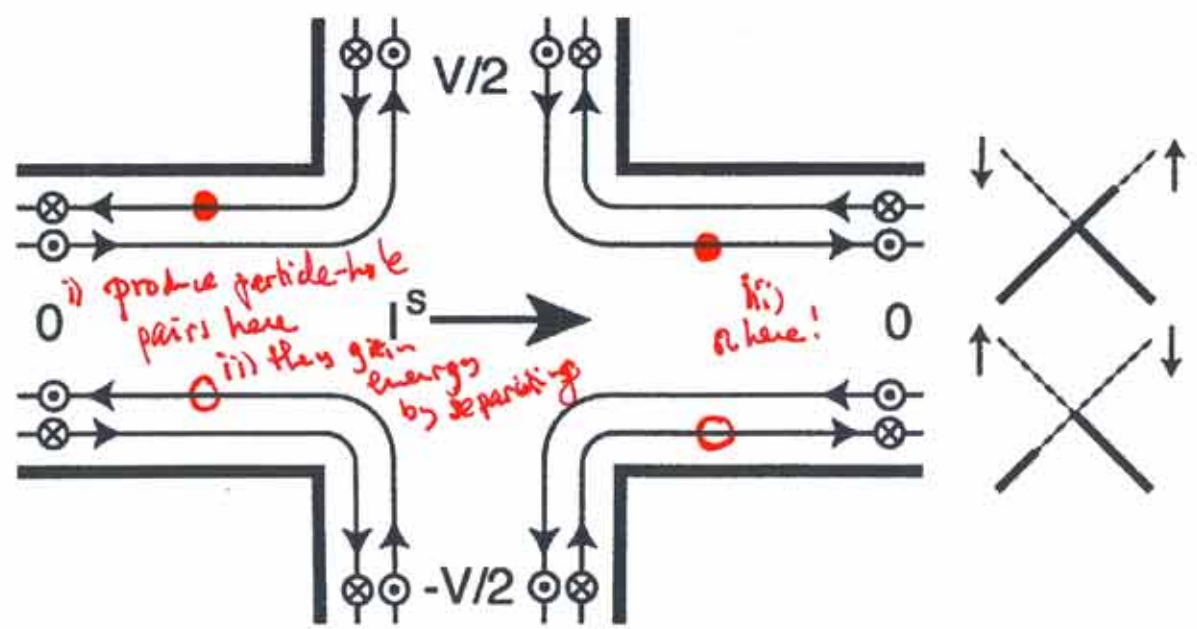


The "sign" of this effect depends on the sign of  $\Delta_{so}$  (a material property).

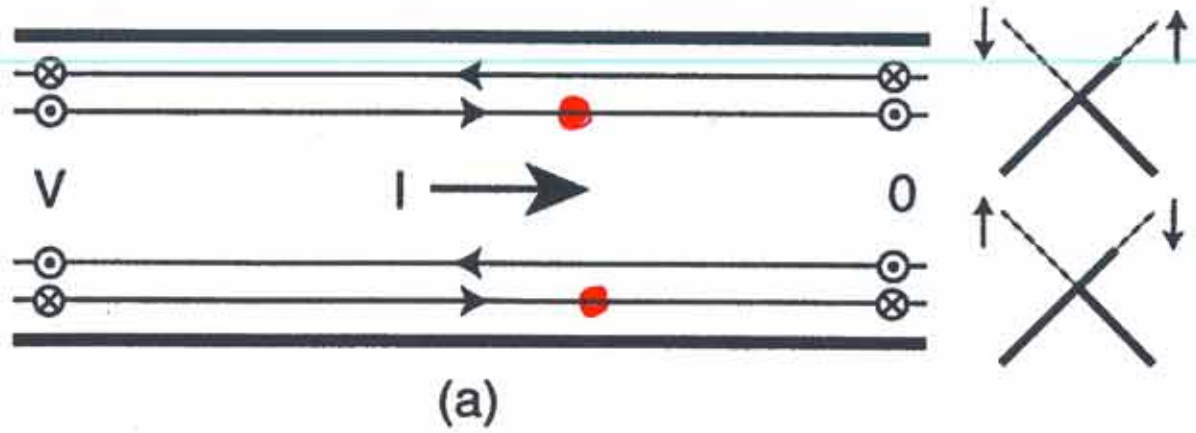
Think dynamically!  
(i.e. Electrons move opposite to currents [Franklin])



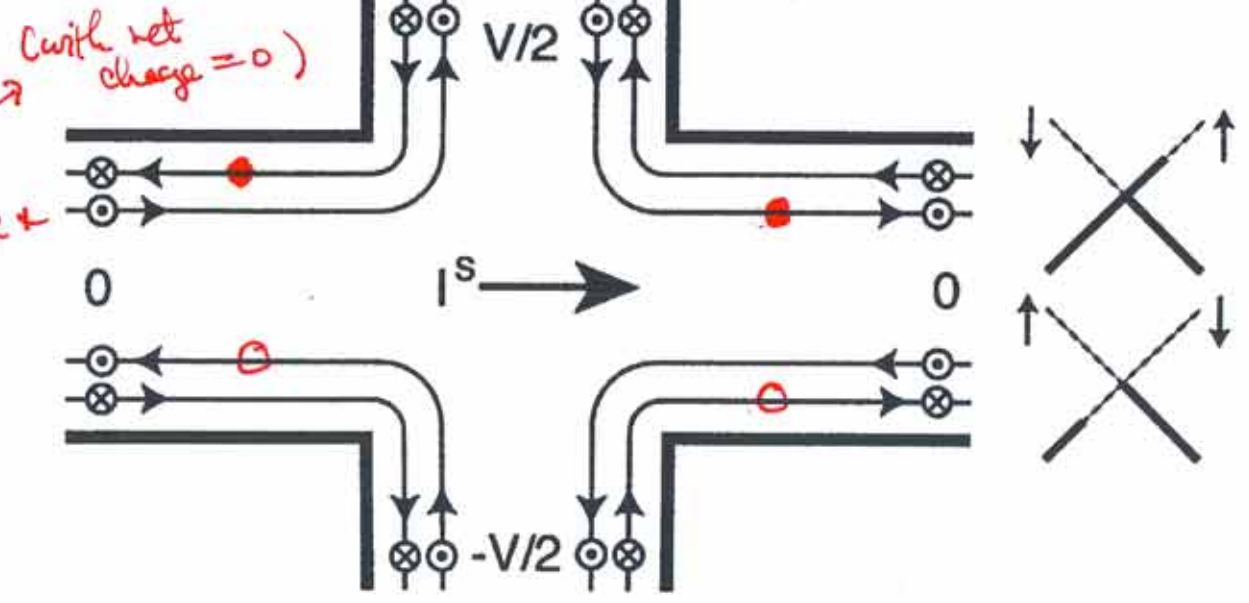
(a)



Net spin accumulates at edges!



Injected spin separates charge + induces voltage!





Scholiens to massless Dirac equation (conjecture)

Emerged by calculation from nearest-neighbor hopping.

Mass (opening of gap) for  $\begin{cases} A \text{ vs. } B \text{ potential} \\ t_2 \sin \phi \neq 0 \text{ (T violation)} \end{cases}$

Conjecture: consequence of  $C_{60} + T$

2d rep. of  $C_{30}$

$E \rightarrow -E$  for  $C_{60}/C_{30} \times T$

This, and transport minimum, need clarification.

↳ [Ziegler PRL 80, 3113]



## 15.3 $Z_2$ Invariant for Quantum Spin Hall

15.21

Kane + Mele cond-mat/0506581

15.3.1 As we've discussed, the critical issue is whether there's an ~~even~~ odd number of Kramers pairs within the bulk gap.

There's a  $Z_2$  topological invariant for T-invariant systems, defined directly in terms of Bloch Hamiltonians, that answers this question.

(N.B. This is over and above the TKNN integers (Chern #s), which do not require - in fact they trivialize for - T-invariant.)

### 15.3.2

On background, for graphene (Haldane's model)

$$H = t \sum_{\langle ij \rangle} c_i^\dagger c_j + i \Delta_{SO} \sum_{\langle\langle ij \rangle\rangle} v_{ij} c_i^\dagger S^z c_j \quad \text{"spin-split"}$$

*N.N. hoppings* (pointing to  $\langle ij \rangle$ )  
*NNN, oriented* (pointing to  $\langle\langle ij \rangle\rangle$ )

$$+ i \lambda_R \sum_{\langle ij \rangle} c_i^\dagger (S \times \hat{d}_{ij})_z c_j + \lambda_\sigma \sum_i \epsilon_i c_i^\dagger c_i$$

*Rashba* (pointing to  $(S \times \hat{d}_{ij})_z$ )  
*A $\leftrightarrow$ B breaking* (pointing to  $\epsilon_i$ )

The Bloch Hamiltonian is

$$H(\vec{k}) = \sum_{a=1}^5 d_a(\vec{k}) T^a + \sum_{a < b=1}^5 d_{ab}(\vec{k}) T^{ab}$$

(4 component spins: 2 for  $\vec{A}$  or  $\vec{B}$  and two for spin  $\vec{S}$ )

$$T^{(1,2,3,4,5)} = (\sigma^x \otimes \mathbb{1}, \sigma^z \otimes \mathbb{1}, \sigma^y \otimes S^x, \sigma^y \otimes S^y, \sigma^z \otimes S^z)$$

$$T^{ab} = \frac{1}{2i} [T^a, T^b]$$

Under time reversal

$$\Theta |u\rangle = i(\mathbb{I} \otimes S^y) |u\rangle^*$$

$$\Theta T^a \Theta^{-1} = T^a \quad ; \quad \Theta T^{ab} \Theta^{-1} = -T^{ab}$$

$H$  is  $T$  symmetric  $\iff d_a(\vec{k}) = d_a(-\vec{k})$  and  $d_{ab}(\vec{k}) = -d_{ab}(-\vec{k})$ .

For Haldane's model:

$d_1$	$t(1 + 2\cos x \cos y)$	$d_{12}$	$-2t \cos x \sin y$
$d_2$	$\lambda v$	$d_{15}$	$\Delta_{50}(2 \sin 2x - 4 \sin x \cos y)$
$d_3$	$\lambda_R (1 - \cos x \cos y)$	$d_{23}$	$-\lambda_R \cos x \sin y$
$d_4$	$-\sqrt{3} \lambda_R \sin x \sin y$	$d_{24}$	$\sqrt{3} \lambda_R \sin x \cos y$
$d_5$	0	others	0

with  $x \equiv k_x a/2$   
 $y \equiv \sqrt{3} k_y a/2$

15.3.3 Consider

15.23

$$P(\vec{k}) = \text{Pf} [\langle u_i(\vec{k}) | \otimes | u_j(\vec{k}) \rangle]$$

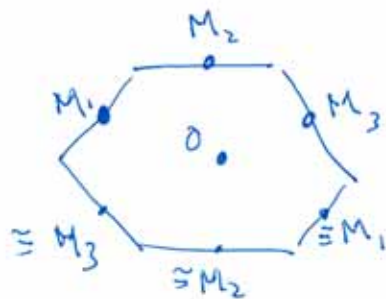
(i.e.  $\langle u_i(\vec{k}) | \otimes | u_j(\vec{k}) \rangle = \epsilon_{ij} P(\vec{k})$ ).

$$\begin{aligned} \Gamma \quad \langle u_i(\vec{k}) | \otimes^3 | u_j(\vec{k}) \rangle &= \langle u_j(\vec{k}) | \otimes | u_i(\vec{k}) \rangle \\ &\stackrel{\text{anti-unitarity}}{=} \\ &= \langle u_i(\vec{k}) | \otimes | u_j(\vec{k}) \rangle \end{aligned}$$

Generically this has isolated zeros (2 parameters, 1 real + 1 complex condition).

The zeros appear in pairs at momenta  $\pm \vec{k}_i$ , with opposite vorticity.

15.3.4 A single pair might annihilate if  $\pm \vec{k}_i \cong -\vec{k}_i$  (i.e., up to a reciprocal lattice vector). That  $\cong$  occurs at  $\vec{k}_i = 0$  or one of the M points:



Canonical equivalence takes  $\psi_1 \rightarrow \psi_1^*$ ,  $\psi_2 \rightarrow -\psi_1^*$ ; others are U(2) rotations of this, and  $\text{Pf}(UM) = \det U \text{Pf} M$

But for a T-invariant system the eigenspaces at these points are equivalent (since  $\otimes H_{\vec{k}}^{\otimes} = H_{-\vec{k}}^{\otimes}$ ) so  $|P(\vec{k})| = 1$ .



15.3.5 Of course, nothing prohibits pairs of pairs (with opposite vorticity) from annihilating. Thus the # of pairs is conserved (against arbitrary T-invariant perturbations) mod 2.

15.3.6 It can be calculated by integrating the phase of  $P$  around  $1/2$  a Brillouin zone!

15.3.7 For  $\lambda_0 = 0$  things are not generic -  $P(k)$  is real, and vanishes along lines. However, a regulated integral (inserting  $\lambda_0!$ ) still defines the ~~invariant~~  $\mathbb{Z}_2$  invariant.

15.3.8 The <sup>direct</sup> connection to transport and to many-body physics should be made explicit. [In the literature, it is heuristic at best.]