

# Quantum Spin Hall Effect And Topological Phase Transition in HgTe Quantum Wells

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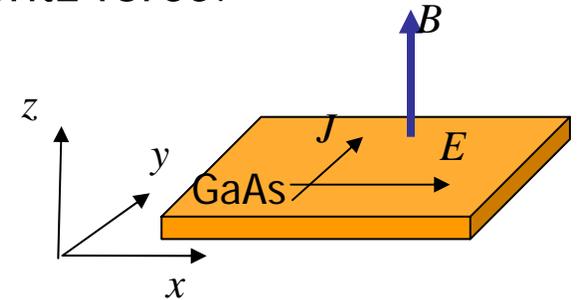
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With: Taylor L. Hughes, Shou-Cheng Zhang (Stanford University)

# Generalization of the quantum Hall effect

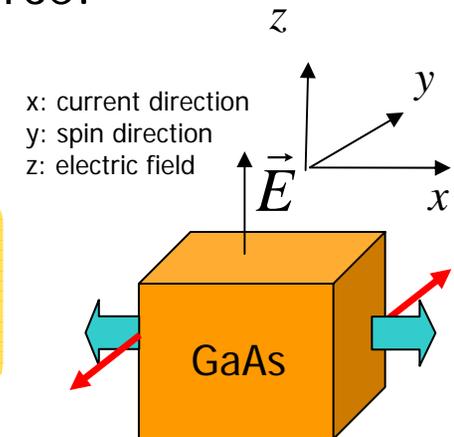
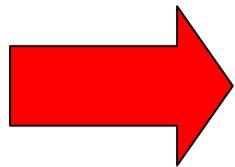
- Quantum Hall effect exists in D=2, due to Lorentz force.

$$J_i = \sigma_H \varepsilon_{ij} E_j \quad \sigma_H = \frac{p e^2}{q h}$$



- Natural generalization to D=3, due to spin-orbit force:

$$J_j^i = \sigma_{spin} \varepsilon_{ijk} E_k \quad \sigma_{spin} \propto ek_F$$



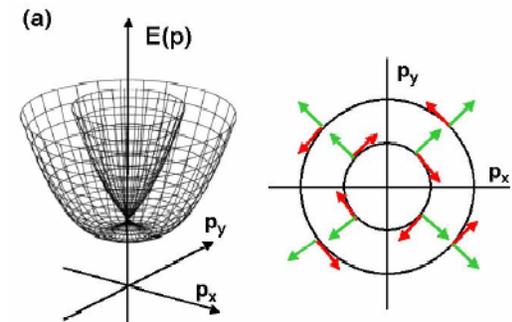
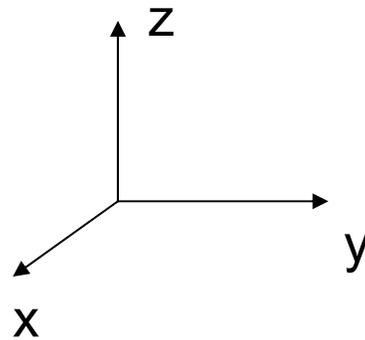
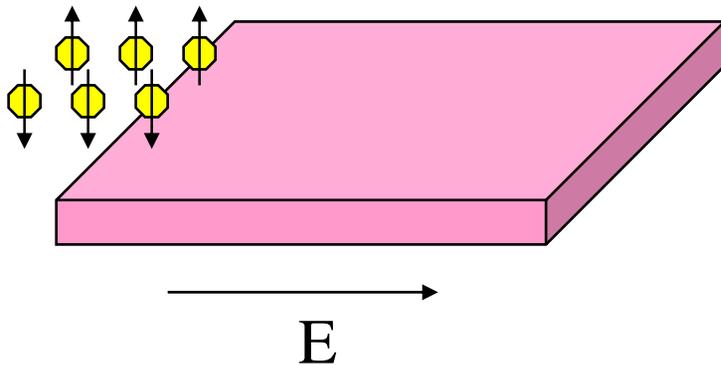
- 2D electron systems (Sinova et al)
- 3D hole systems (Murakami et al)

# Response to Electric Field

- 2D electron systems (Sinova et al)
- 3D hole systems (Murakami et al)

$$j_j^i = \sigma_I \epsilon_{ijk} E_k$$

Suppose  $E$  in  $y$ -direction. Then there will be a spin current flowing in the  $x$ -direction with spins polarized in the  $z$ -direction.

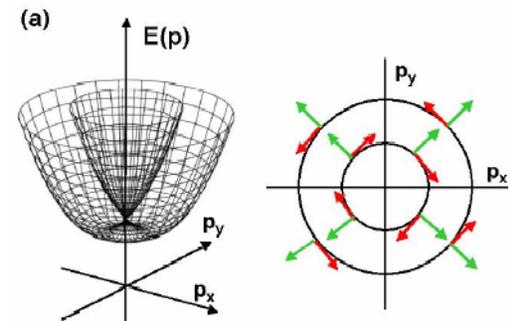
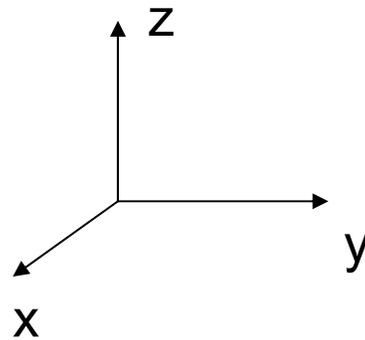
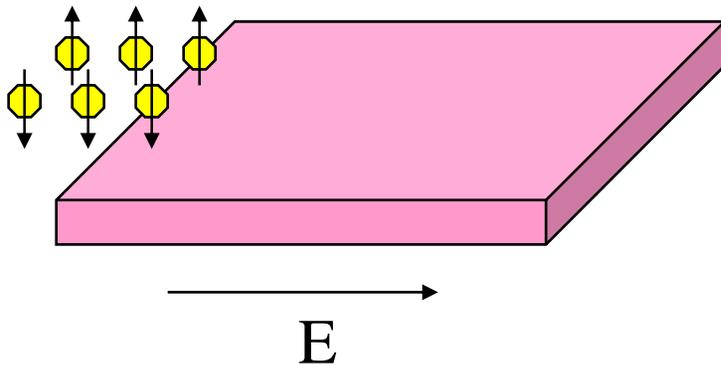


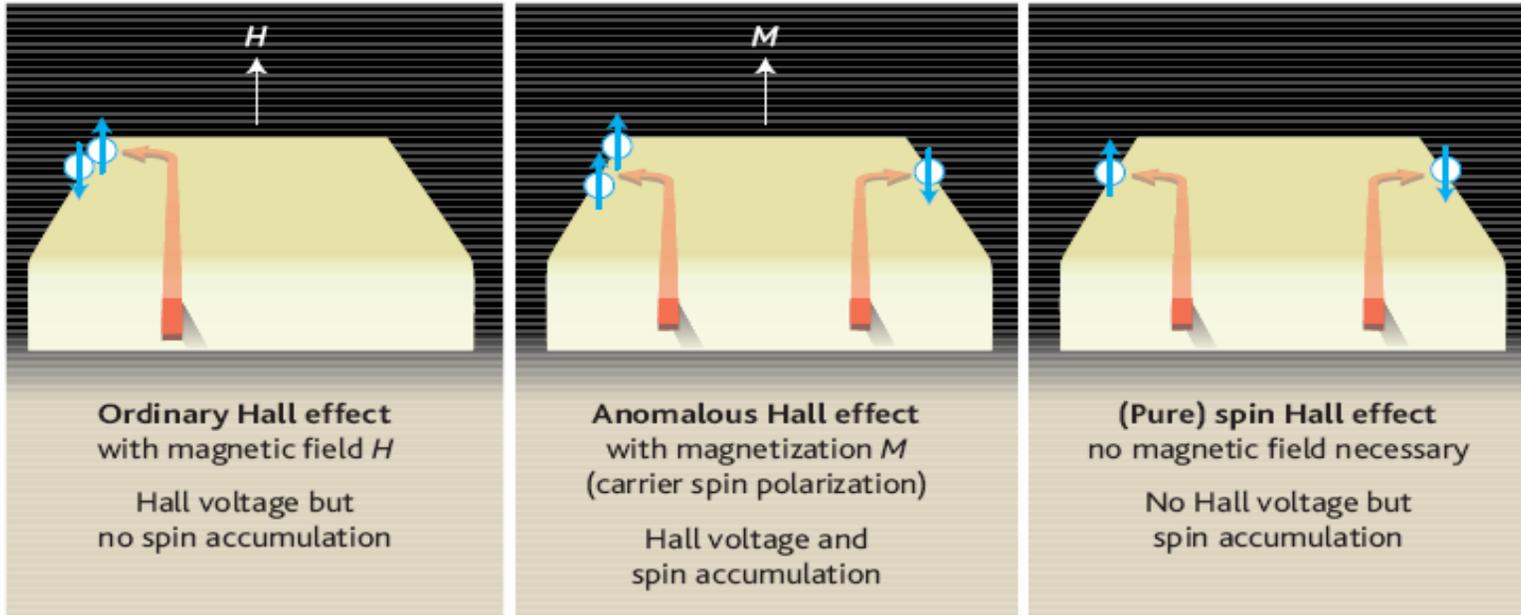
# Response to Electric Field

$$j_j^i = \sigma_I \epsilon_{ijk} E_k$$

No net charge flow since the same number of electrons flow in each direction.

Since system has Fermi surface it dissipates, has longitudinal resistivity

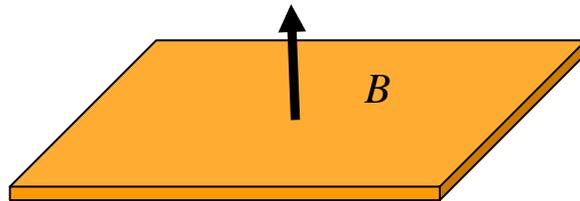




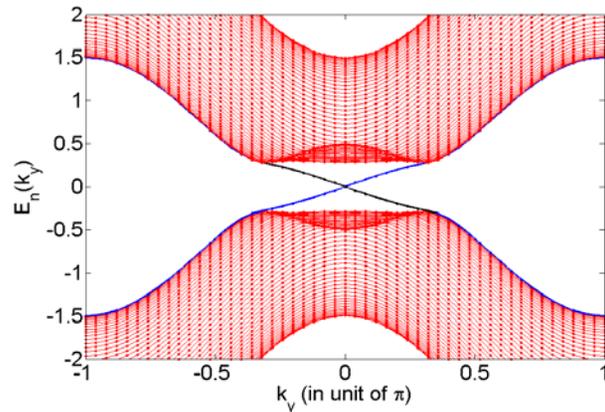
How about quantum spin Hall?

# Quantum Hall Effect

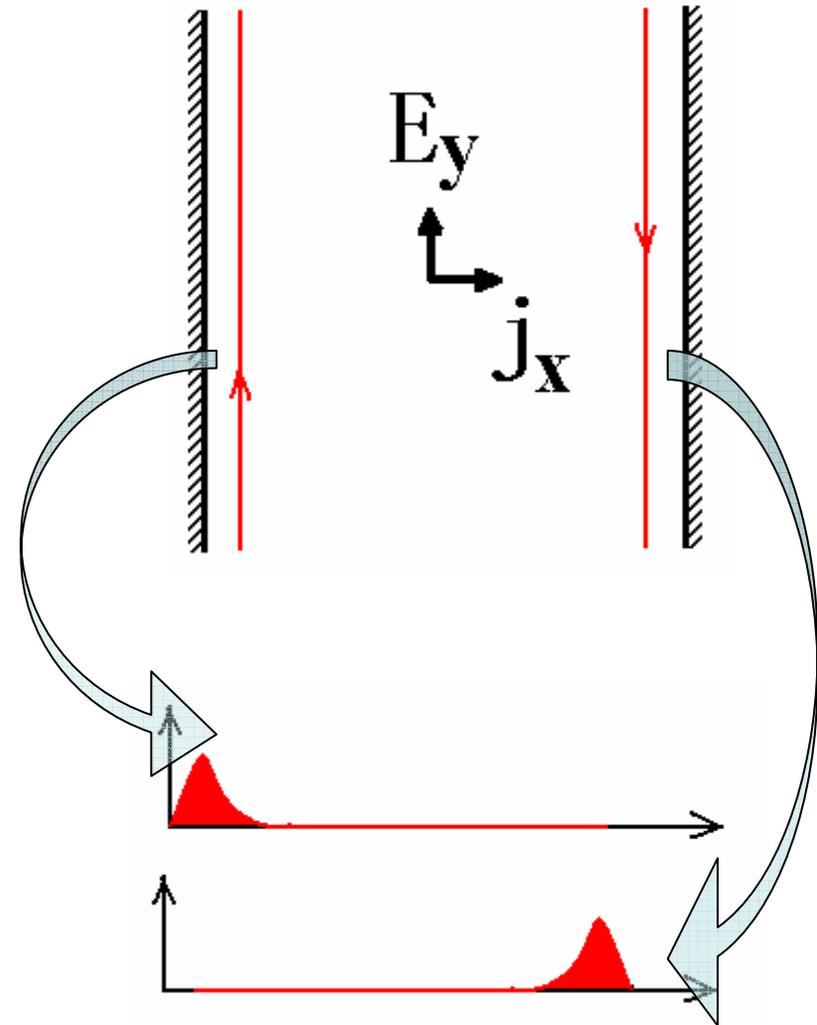
With Applied Magnetic Field



Without Applied Magnetic Field,  
with intrinsic T-breaking  
(magnetic semiconductors)



First proposed model in graphene  
(Haldane, PRL 61, 2015 (1988));



# Quantum Anomalous Hall Effect

Qi et al, 2006

Magnetic semiconductor with SO coupling (no Landau levels):

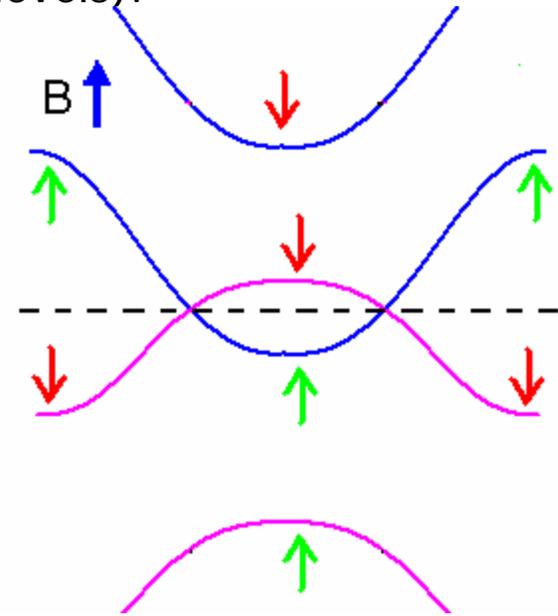
General 2×2  
Hamiltonian

$$H = \epsilon(k) + V d_a(k) \sigma^a$$

Example

$$H = -t \sum_{\langle ij \rangle} (c_i^\dagger c_j + h.c.)$$

$$- \frac{V}{2} \sum_{\langle ij \rangle} (c_i^\dagger \sigma^z c_j + h.c.) + \lambda \sum_i c_i^\dagger \sigma^z c_i$$



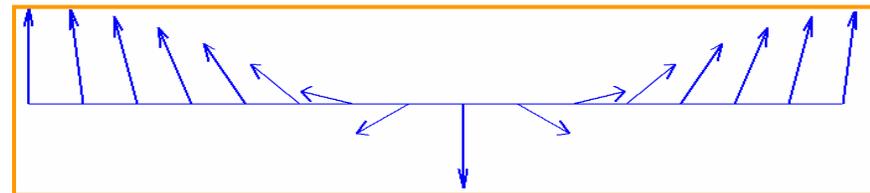
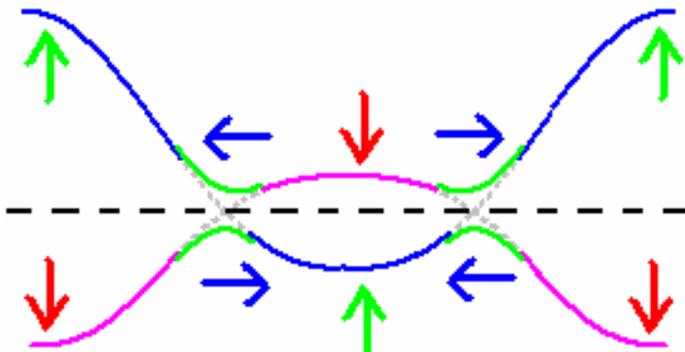
# Quantum Anomalous Hall Effect

Hall Conductivity

$$H = \epsilon(\mathbf{k}) + V d_\alpha(\mathbf{k}) \sigma^\alpha$$



$$\sigma_{ij} = \frac{1}{2\Omega} \sum_{\mathbf{k}} \frac{\partial \hat{d}_\alpha(\mathbf{k})}{\partial k_i} \frac{\partial \hat{d}_\beta(\mathbf{k})}{\partial k_j} \hat{d}_\gamma \epsilon^{\alpha\beta\gamma} (n_+ - n_-)(\mathbf{k}).$$

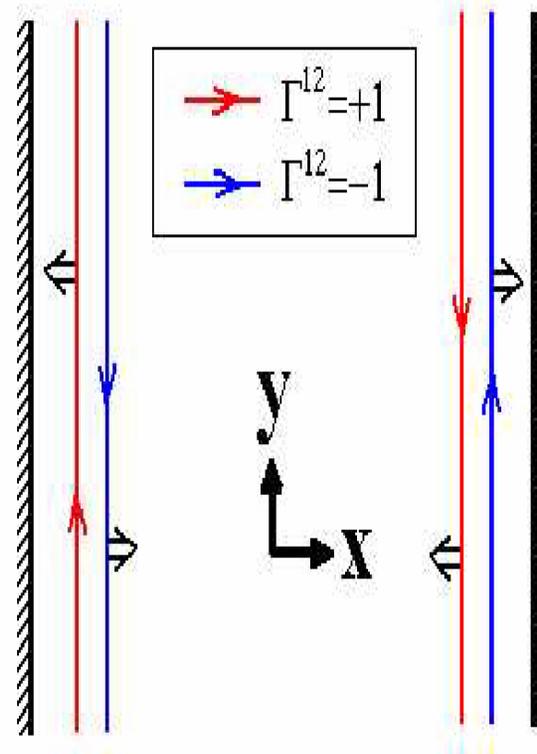
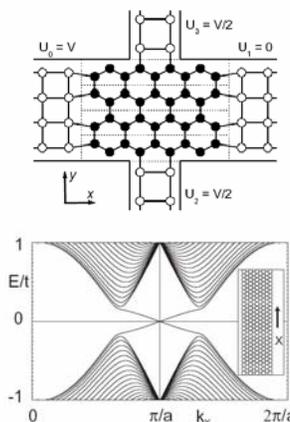


# Quantum Spin Hall Effect

- Physical Understanding: Edge states

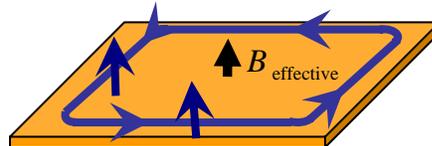
Without Landau Levels,  
(non-magnetic semiconductors  
with Spin-Orbit coupling)

Graphene, Topological Semicond  
by correlating the Haldane model with  
spin (Kane and Mele, PRL (2005),  
Qi, Wu, Zhang PRB (2006));

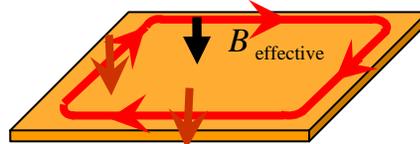


With Landau Levels correlated  
with spin through SO coupling  
(Bernevig and Zhang, PRL (2006));

$$\phi_n = \frac{z^n}{\sqrt{\pi n!}} e^{-\frac{1}{2}zz^*}$$



$$\phi_m = \frac{(z^*)^m}{\sqrt{\pi m!}} e^{-\frac{1}{2}zz^*}$$



- (Sheng et al, PRL, (2005);
- Kane and Mele PRL, (2005);
- Wu, Bernevig and Zhang PRL (2006);
- Xu and Moore PRB (2006) ...

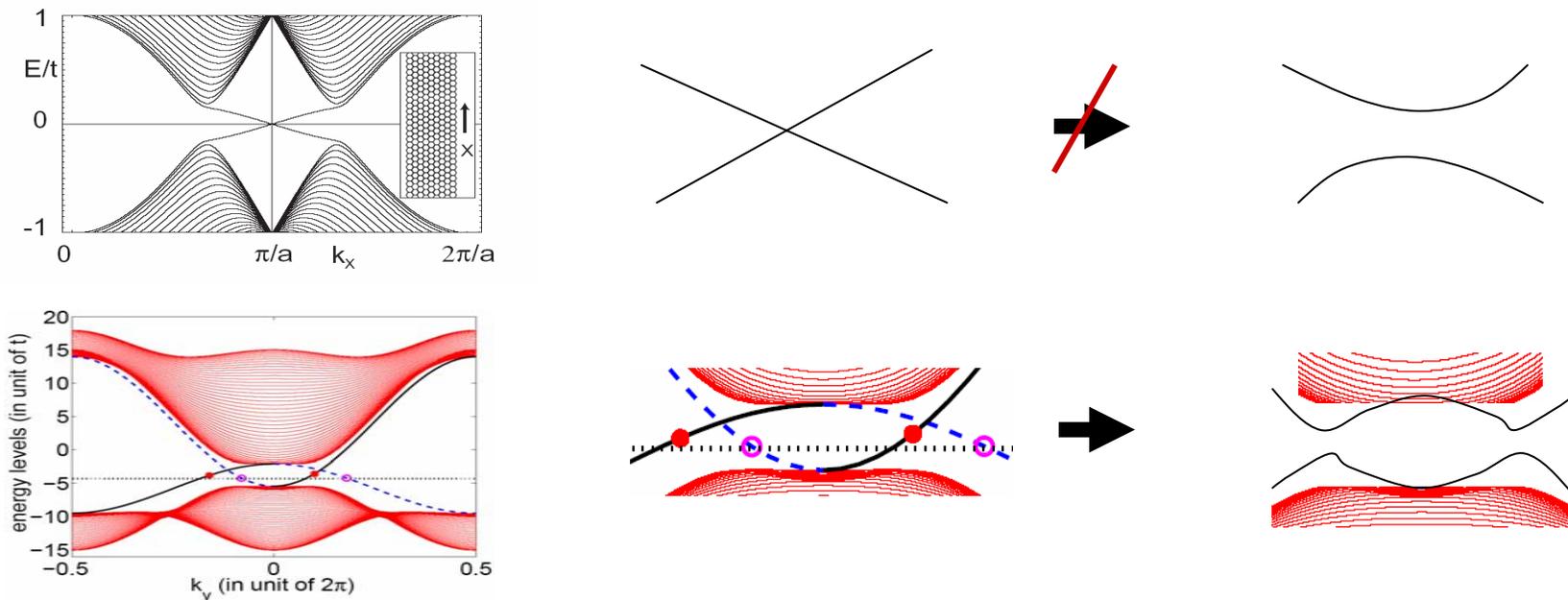
## Z2 Topological classification

- Number of edge state PAIRS on each edge must be odd

Kane and Mele PRL, (2005);

- Single particle backscattering not TR invariant – not allowed
- Umklapp relevant for  $K < 1/2$ , opens gap for strong interactions.

Wu, Bernevig and Zhang PRL (2006);



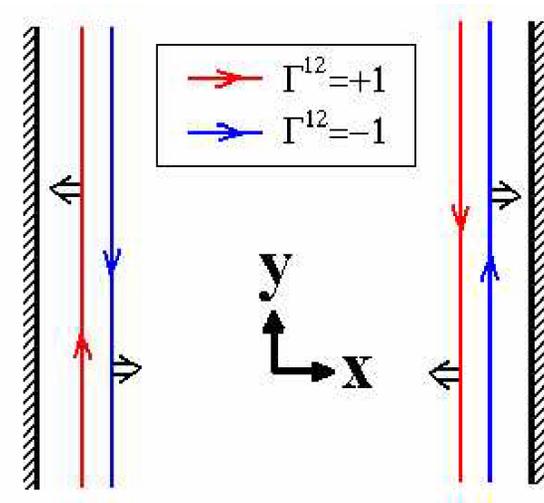
## Helical Liquid - Edge Liquid

- The edge states of the QSHE is the 1D helical liquid. Opposite spins have the opposite chirality at the same edge.

- It is different from the 1D chiral liquid (T breaking), and the 1D spinless fermions.

$$T = e^{i\pi S_y} \quad T^2 = e^{2i\pi S_y}$$

- $T^2=1$  for spinless fermions and  $T^2=-1$  for helical liquids.



$$T\Psi_{R\uparrow}T^{-1} = \Psi_{L\downarrow} \quad T\Psi_{L\downarrow}T^{-1} = -\Psi_{R\uparrow}$$

$$T(\Psi_{R\uparrow}^+\Psi_{L\downarrow} + \Psi_{L\downarrow}^+\Psi_{R\uparrow})T^{-1} = -(\Psi_{R\uparrow}^+\Psi_{L\downarrow} + \Psi_{L\downarrow}^+\Psi_{R\uparrow})$$

- Single particle backscattering is not possible for helical liquids with odd number of fermion pairs!

$$\psi_{1R\uparrow}^\dagger \psi_{2L\downarrow} - \psi_{1R\downarrow}^\dagger \psi_{2R\uparrow} + h.c.$$

## Helical Liquid - Edge of Quantum Spin Hall

- Single particle backscattering not TR invariant – not allowed
- Bosonize Umklapp, assume  $g_u < 0$ . Umklapp relevant for  $K < 1/2$

$$\mathcal{H} = \int dx \frac{v}{2} \left\{ \frac{1}{K} (\partial_x \phi)^2 + K (\partial_x \theta)^2 \right\} + \frac{g_u \cos \sqrt{16\pi} \phi}{2(\pi a)^2}$$

$$\phi = 0, \frac{\sqrt{\pi}}{2} \quad O_2 = i(\psi_{R\uparrow}^\dagger \psi_{L\downarrow} - h.c.) \sim \cos \sqrt{4\pi} \phi \rightarrow O_2 = \pm 1$$

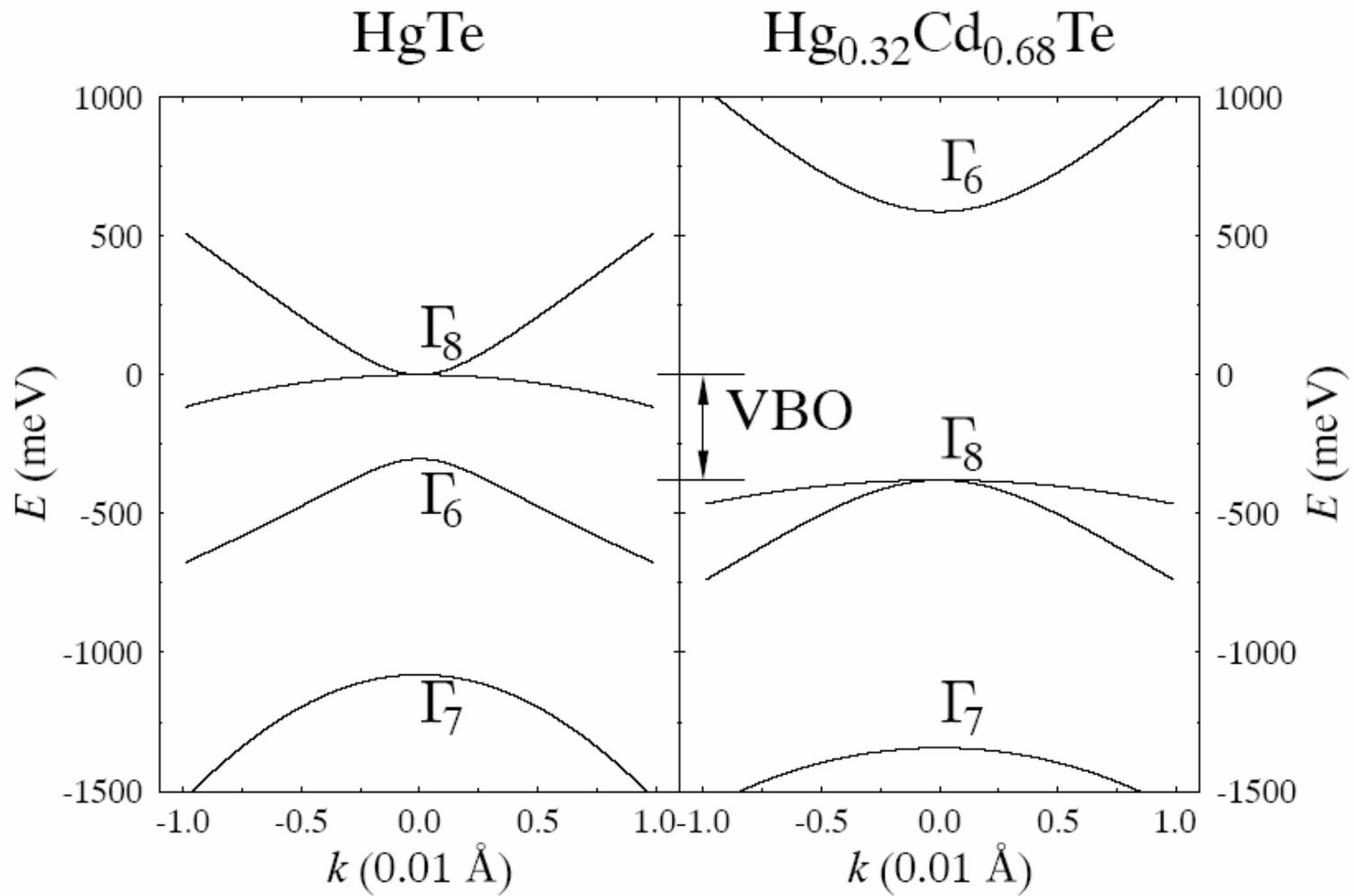
- Ising – like. Ordered at  $T=0$  and TR broken; For  $T > 0$ , Ising disorders. Mass gap with restored TR kills QSHE, only for strong interactions
- A QSHE with even number of electron pairs for one edge is easy to open a TR invariant gap. For  $n=2$  pairs:

$$\psi_{1R\uparrow}^\dagger \psi_{2L\downarrow} - \psi_{1L\downarrow}^\dagger \psi_{2R\uparrow} + h.c.$$

# Quantum Spin Hall Effect

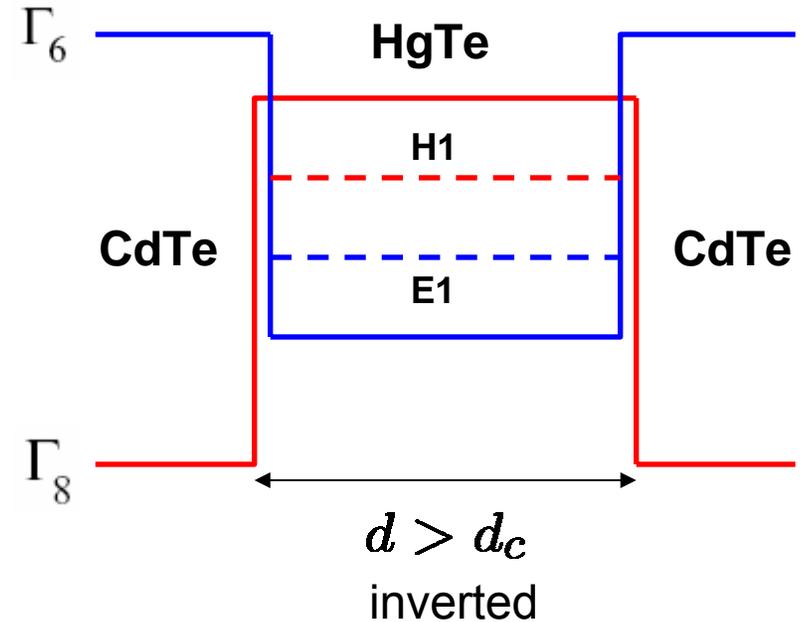
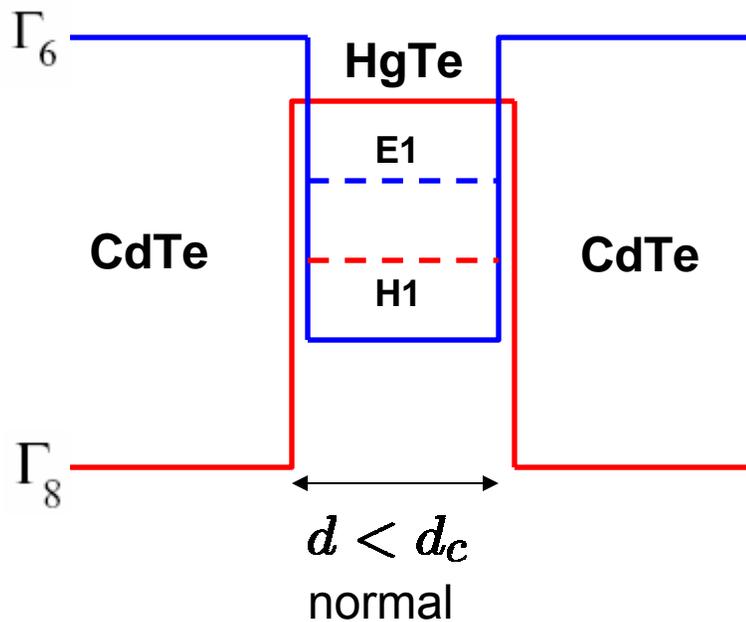
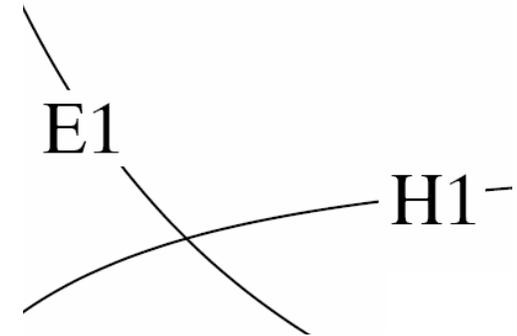
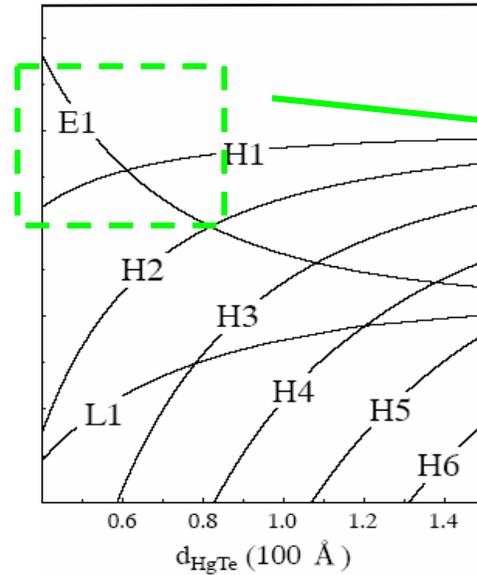
- Graphene – spin-orbit coupling almost inexistent. Even so, no reliable way of telling whether on Spin Hall or trivial insulator side
- Quantum spin Hall with Landau levels – too small spin-orbit coupling, unrealistic
- Conceptual problem to theoretically find materials with QSH state of matter
- Need tight-binding model.
- Have only reliable  $k_p$  perturbation theory
- Goal: finding the QSHE state of matter in some material

# Bulk Band Structure



# Quantum Well Sub-bands

Let us focus on  
E1(s-wave),  
H1(p-wave)  
bands close to  
crossing point



# Envelope Functions

$$\Psi(k_x, k_y, z) = e^{i(k_x x + k_y y)} \begin{pmatrix} f_1(z) \\ f_2(z) \\ f_3(z) \\ f_4(z) \\ f_5(z) \\ f_6(z) \end{pmatrix} \begin{matrix} \Gamma_6, +\frac{1}{2} \\ \Gamma_6, -\frac{1}{2} \\ \Gamma_8, +\frac{3}{2} \\ \Gamma_8, +\frac{1}{2} \\ \Gamma_8, -\frac{1}{2} \\ \Gamma_8, -\frac{3}{2} \end{matrix}$$

$$\psi_{1,\dots,4} = (|E1, + \rangle, |H1, + \rangle, |E1, - \rangle, |H1, - \rangle)$$

Colors indicate non-zero components for each band at  $k=0$

Effective Hamiltonian E1, H1 bands close to crossing point

$$H_{ij}^{eff}(k_x, k_y) = \int_{-\infty}^{\infty} dz \langle \psi_j | \mathcal{H}(k_x, k_y, -i\partial_z) | \psi_i \rangle$$

$\mathcal{H}(k_x, k_y, -i\partial_z)$  is the Kane  $6 \times 6$  Hamiltonian, we neglect the split-off band.

# Effective 4-band Model

$$H_{eff}(k_x, k_y) = \begin{pmatrix} H & 0 \\ 0 & H^* \end{pmatrix}, \quad H = \epsilon(k) + d_i(k)\sigma_i$$

$$d_1 + id_2 = A(k_x + ik_y) \equiv Ak_+$$

$$d_3 = M - B(k_x^2 + k_y^2), \quad \epsilon_k = C - D(k_x^2 + k_y^2)$$

Two copies of Massive Dirac Equation with opposite masses  
plus an additional kinetic energy term

A,B,C,D,M are numerical parameters that depend on the well thickness

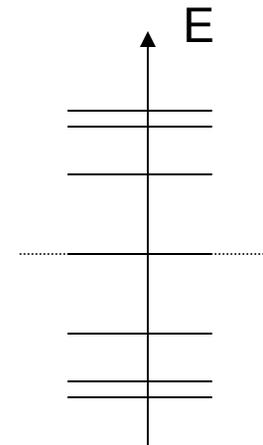
# Continuum Picture

Each diagonal block Hamiltonian has a parity-anomaly  
One Dirac point per spin versus two Dirac point in the graphene model.  
Expect a quantized response from each block of the form:

$$\sigma_{xy} = -\frac{1}{8\pi^2} \int \int dk_x dk_y \hat{\mathbf{d}} \cdot \partial_x \hat{\mathbf{d}} \times \partial_y \hat{\mathbf{d}}$$

$$\sigma_{xy} = \frac{1}{2} \text{sign}(M)$$

For each block spin (they have opposite masses)

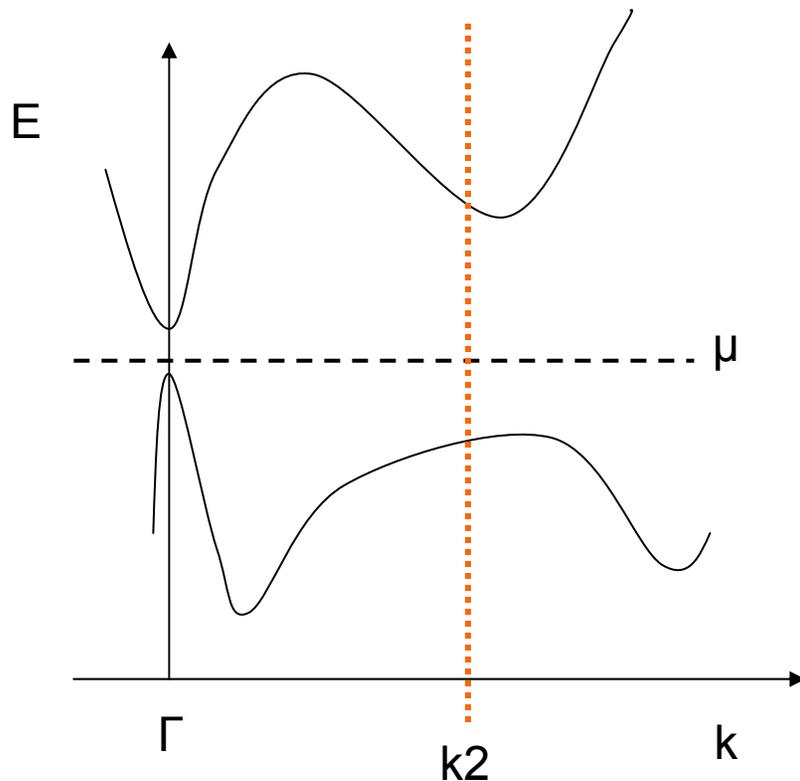


But this gives fractional quantum-Hall conductance for each block, so what is missing?

The Skyrmion number changes by +1 for spin up and -1 for spin down as the Dirac mass term is tuned across zero. The change is what we need!

# Contributions from Brillouin Zone

Look in one of the Dirac blocks, say for spin up



From  $\Gamma$  point we get the contribution:

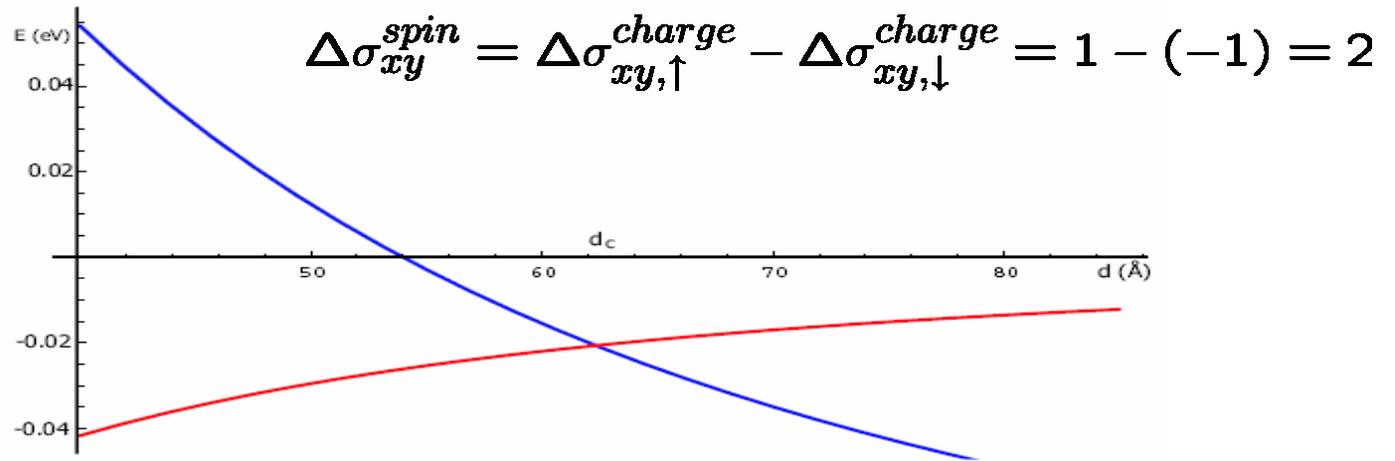
$$\sigma_{xy} = \frac{1}{2} \text{sign}(M)$$

There is a “spectator fermion”,  
generically in a higher energy part of  
BZ:

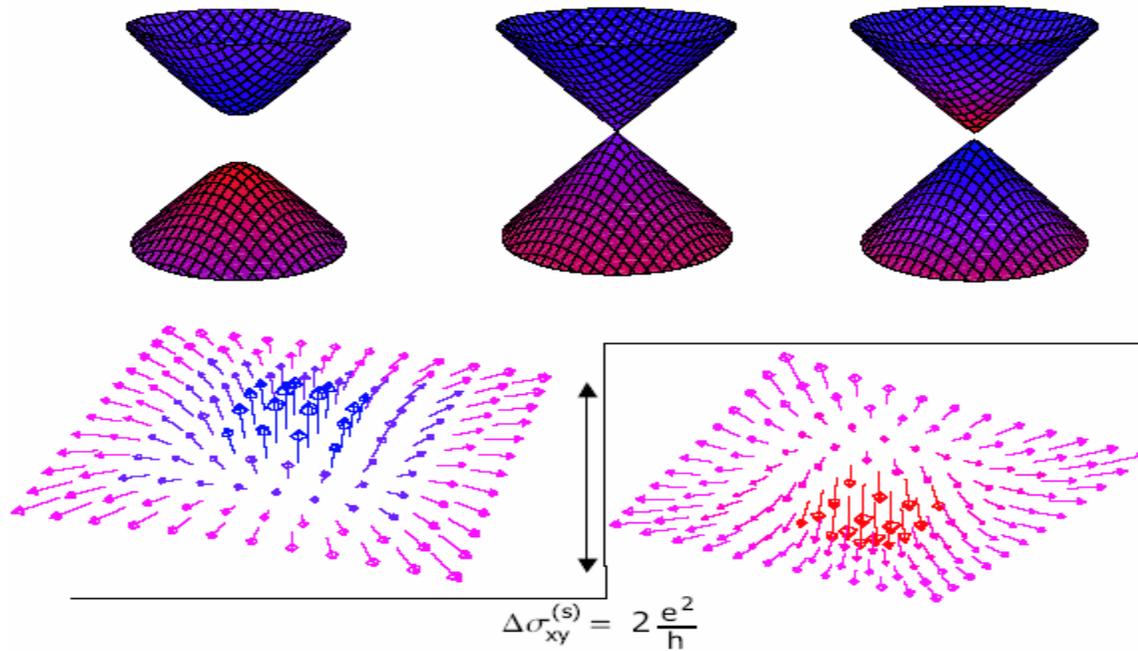
$$\sigma_{xy} = \frac{1}{2} \text{sign}(M_2)$$

Does this add to the contribution at  $\Gamma$  or cancel it? Cannot know unless full BZ structure known, not only low-energy.

# Physical Picture



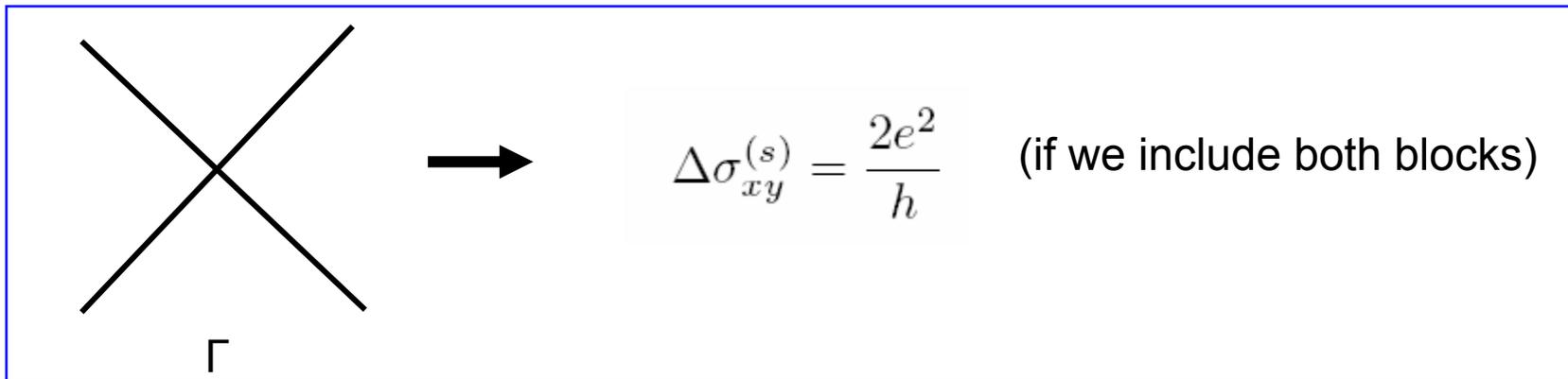
Meron in continuum picture:



# Change in Spin Hall Conductance

From k.p we cannot determine this since we only know about the  $\Gamma$  point

But the gap closes at the  $\Gamma$  point at some specific quantum well thickness. We can determine change in Hall conductance only



→  $[\Delta(\# \text{ of pairs of edge states})] \bmod 2 = 1$  → QSHE exists on one side of transition

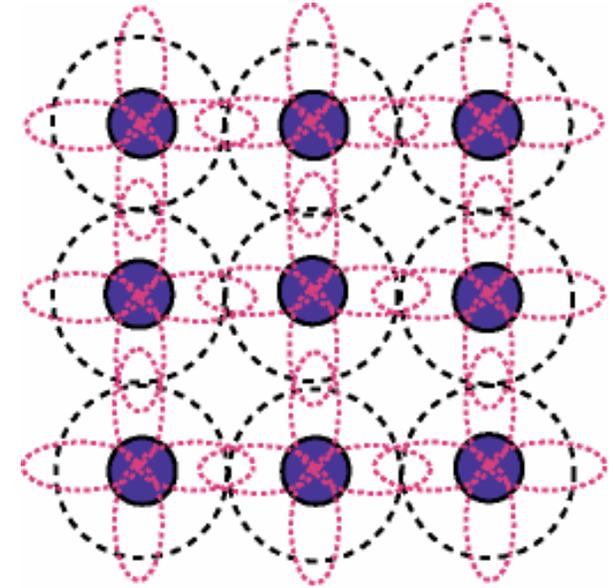
But which side?

# Effective tight-binding model

Square lattice with 4-orbitals per site:

$$|s, \uparrow\rangle, |s, \downarrow\rangle, |(p_x + ip_y), \uparrow\rangle, |-(p_x + ip_y), \downarrow\rangle$$

Consider only the nearest neighbor hopping integrals. Mixing matrix elements between the s and the p states must be odd in k.



$$H_{eff}(k_x, k_y) = \begin{pmatrix} H & 0 \\ 0 & H^* \end{pmatrix}, \quad H = \epsilon(k) + d_i(k)\sigma_i$$

$$\mathcal{H}(k) = \begin{pmatrix} \mathcal{M}(k) & A(\sin(k_x) - i \sin(k_y)) \\ A(\sin(k_x) + i \sin(k_y)) & -\mathcal{M}(k) \end{pmatrix} = d_a(k)\sigma^a \quad a = 1, 2, 3$$

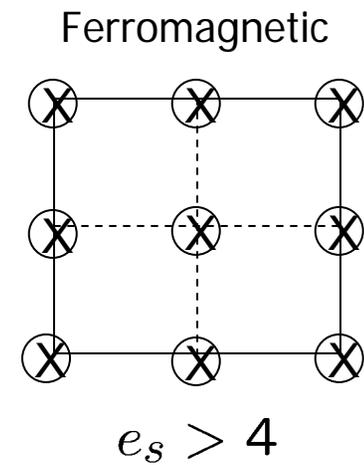
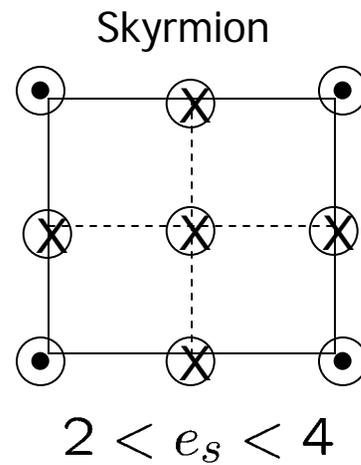
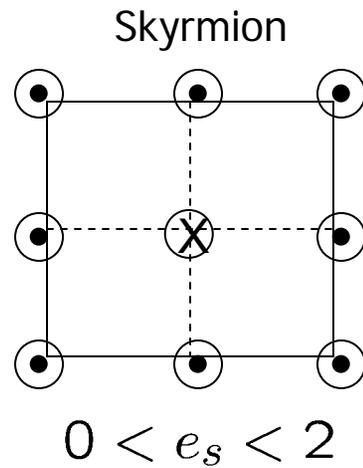
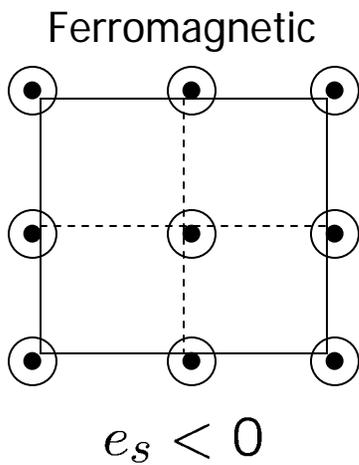
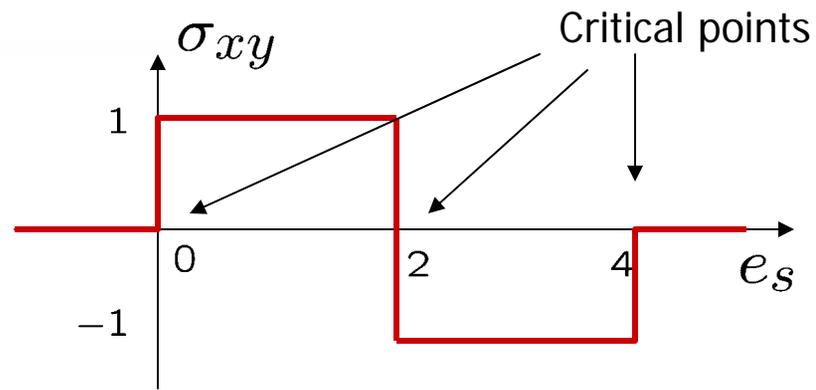
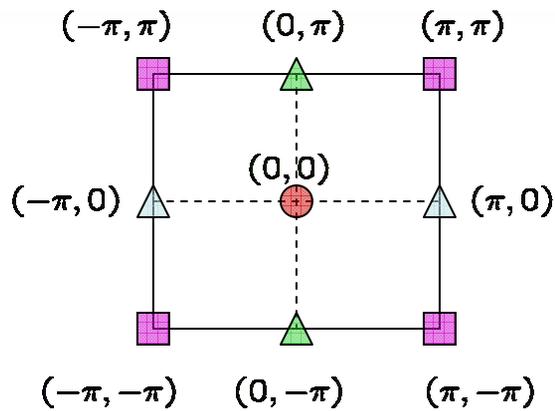
$$\mathcal{M}(k) = -2B\left(2 - \frac{M}{2B} - \cos(k_x) - \cos(k_y)\right), \quad d_1 = A \sin(k_x), \quad d_2 = A \sin(k_y), \quad \text{and} \quad d_3 = \mathcal{M}(k)$$

| $d$ (Å) | $A$ (eV) | $B$ (eV) | $C$ (eV) | $D$ (eV) | $M$ (eV) |
|---------|----------|----------|----------|----------|----------|
| 58      | -3.62    | -18.0    | -0.0180  | -0.594   | 0.00922  |
| 70      | -3.42    | -16.9    | -0.0263  | 0.514    | -0.00686 |

# Topology of the tight-Binding Model

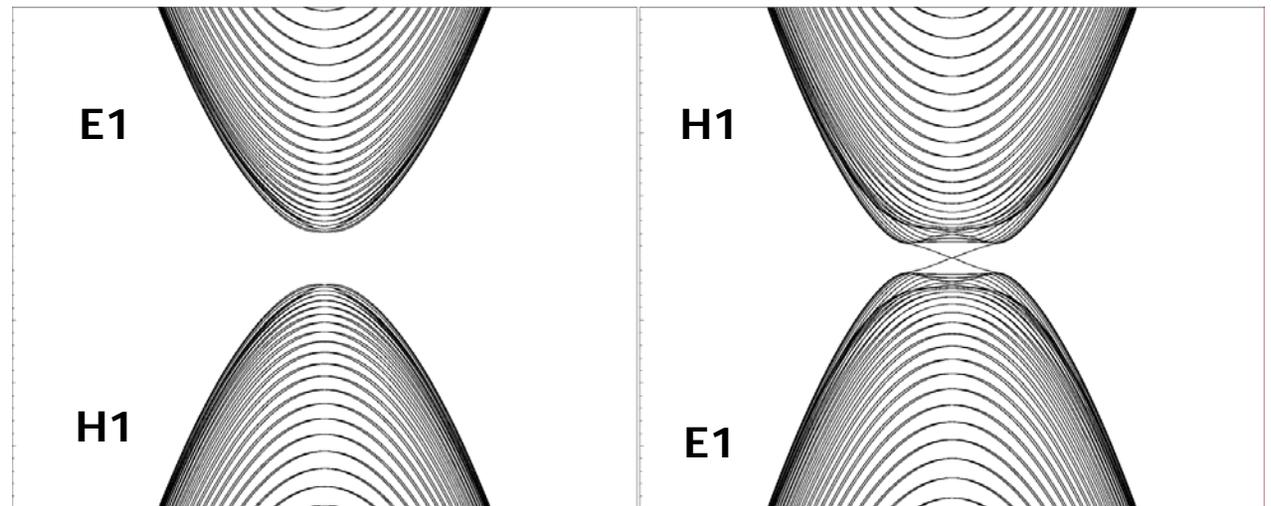
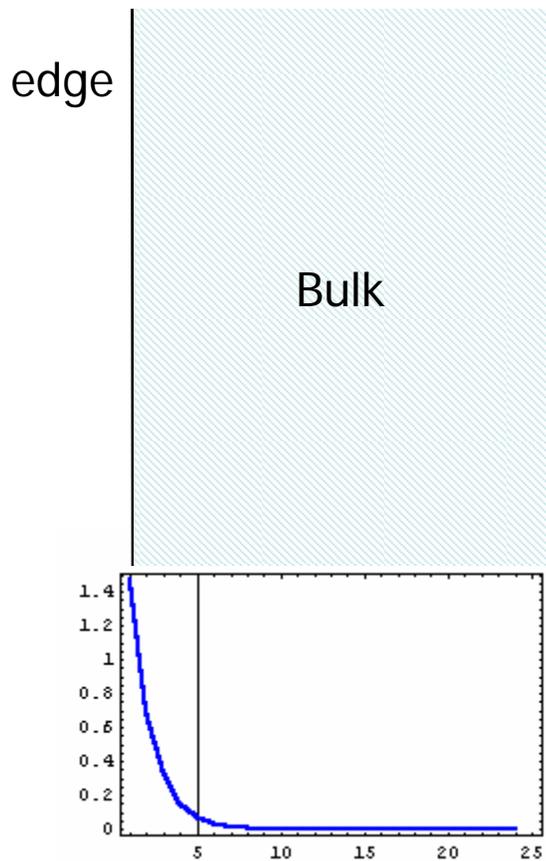
$$d_3 = -2B\left(2 - \frac{M}{2B} - \cos(k_x) - \cos(k_y)\right)$$

$$e_s = \frac{M}{2B}$$



# Edge states of the effective tight-binding model

We can analytically find chiral/anti-chiral edge state solutions which lie in the bulk insulating gap:  $\sigma^y \psi = \pm \psi$

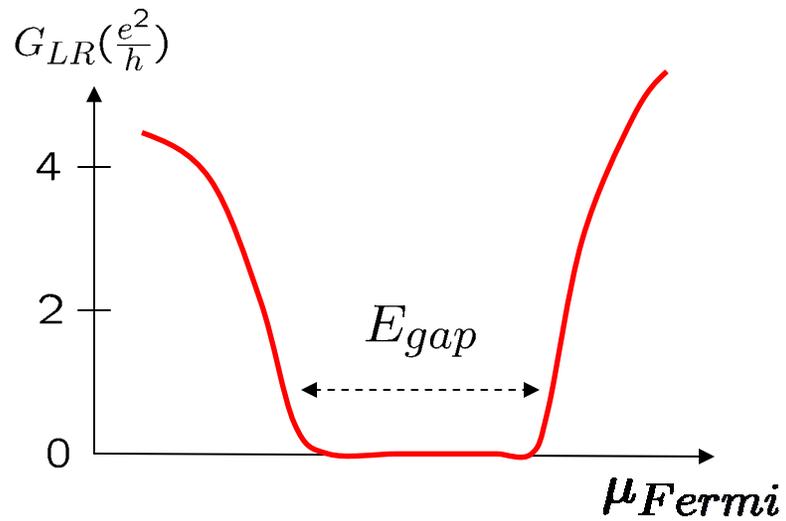


Trivial

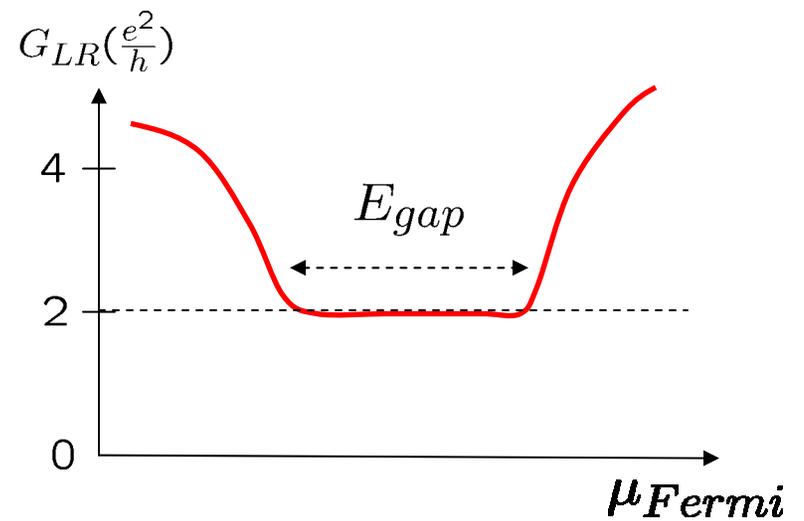
Non-trivial

(neglecting kinetic energy term)

# Experimental Signature (2-terminal)

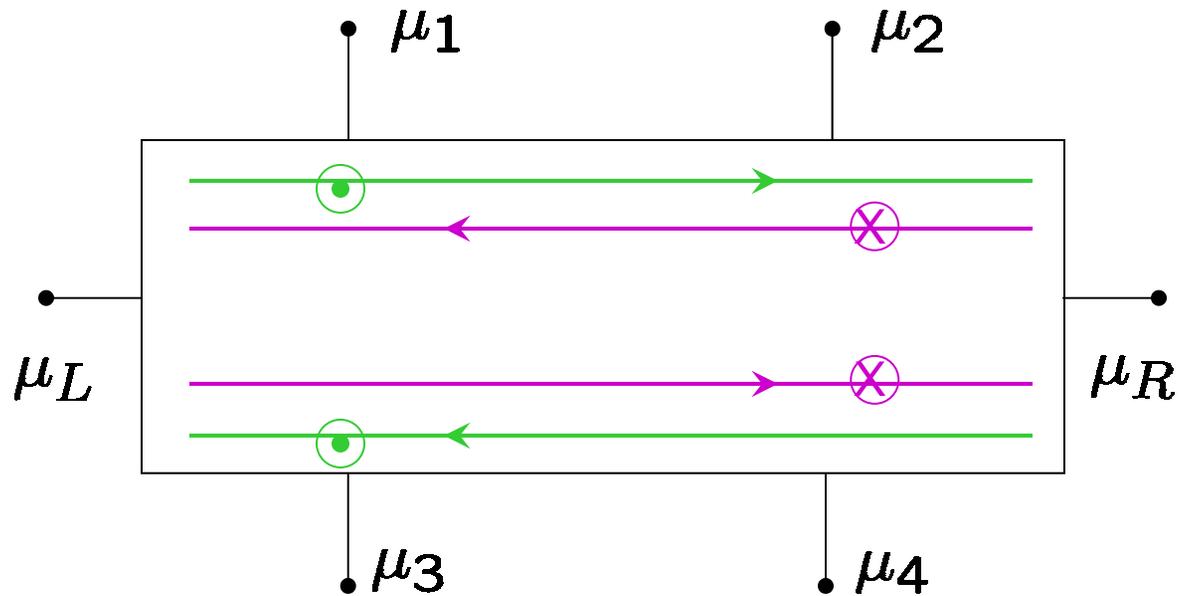


$d < d_c$ , normal regime



$d > d_c$ , inverted regime

# Experimental Signature (6-terminal)



A source-drain current  $j_{LR}$   $\longrightarrow$   $\mu_1 = \mu_2$   
 $\mu_3 = \mu_4$

# Smoking gun for the helical edge state: Magneto-Conductance

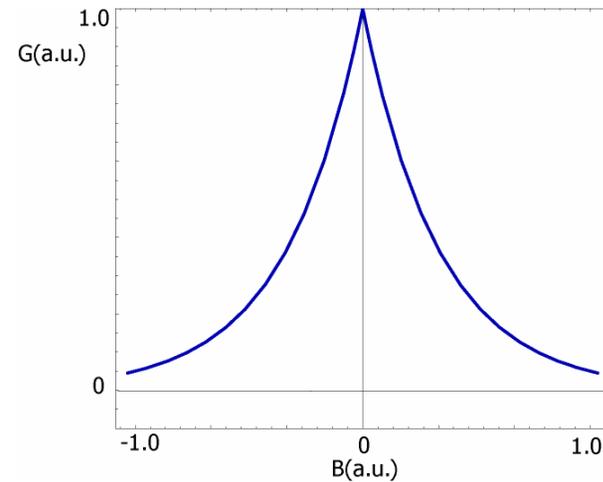
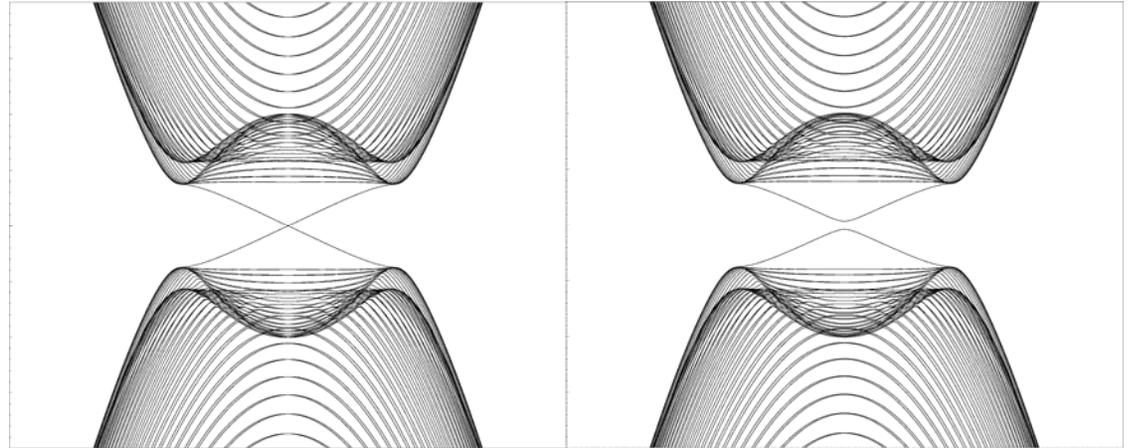
With C. Wu

The crossing of the helical edge states is protected by the TR symmetry. TR breaking term such as the Zeeman magnetic field causes a singular perturbation and will open up a full insulating gap:

$$E_g \propto g|B|$$

Conductance now takes the activated form:

$$\sigma \propto f(T)e^{-g|B|/kT}$$



# Conclusions

- QSH state is a new state of matter, topologically distinct from the conventional insulators.
- It is predicted to exist in HgTe quantum wells, in the "inverted" regime, with  $d > 6$  nm.
- Clear experimental signatures predicted.
- Experimental realization possible.

