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

B. Andrei Bernevig

Princeton Center for Theoretical Physics

Taylor L. Hughes, Shou-Cheng Zhang

Stanford University

Asilomar, June 2007

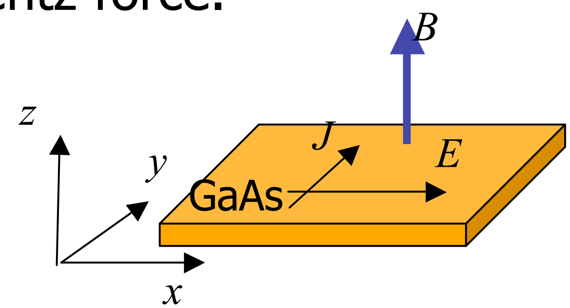
Presented at the PITP/SpinAps Asilomar Conference in June 2007

Brought to you by PITP (www.pitp.phas.ubc.ca)

Generalization of the quantum Hall effect

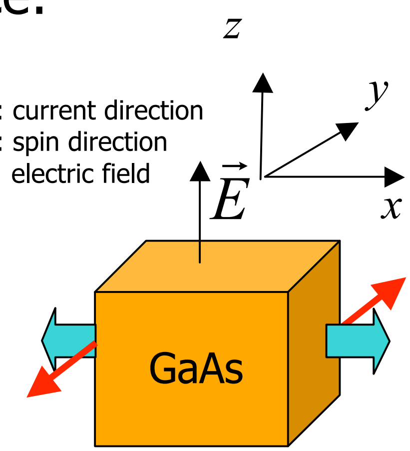
- Quantum Hall effect exists in D=2, due to Lorentz force.

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



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

$$J_j^{\,i} = \sigma_{spin} \varepsilon_{ijk} E_k \qquad \sigma_{spin} \propto e k_F$$

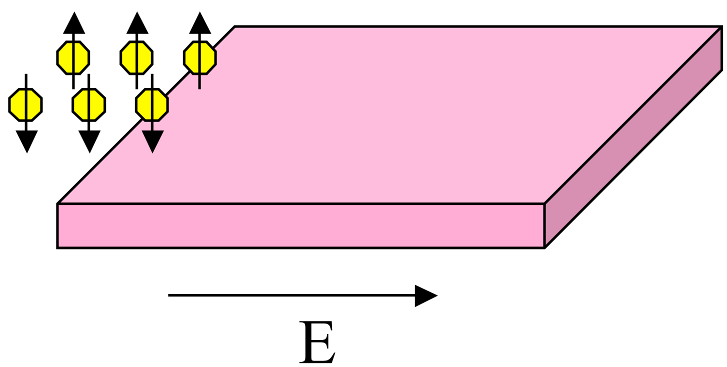


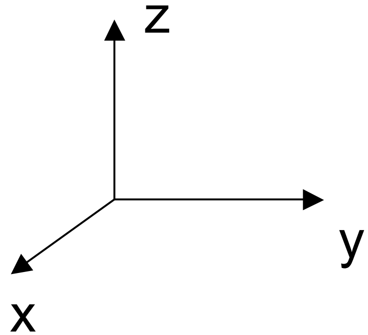
- 3D hole systems (Murakami et al, Science, PRB)
- 2D electron systems (Sinova et al, PRL)

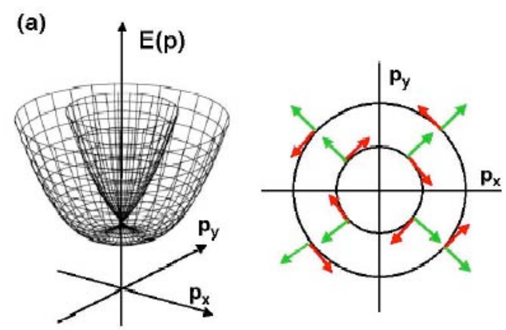
Response to Electric Field

$$j^i_j = \sigma_I \, \epsilon_{ijk} E_k$$

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





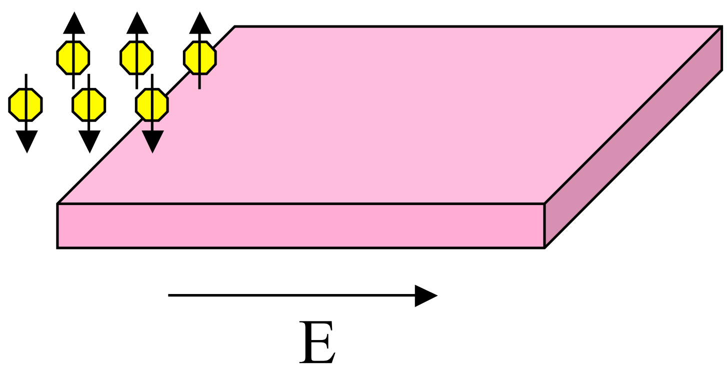


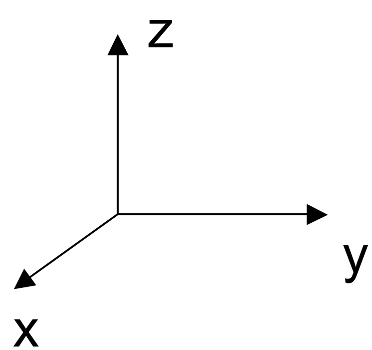
Response to Electric Field

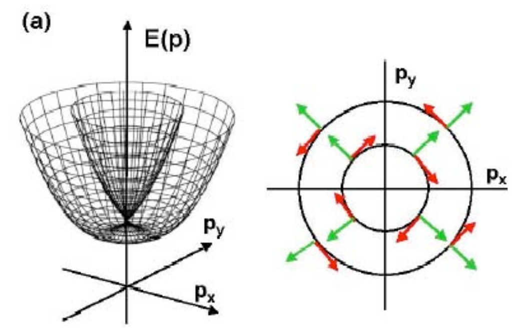
$$j^i_j = \sigma_I \, \epsilon_{ijk} E_k$$

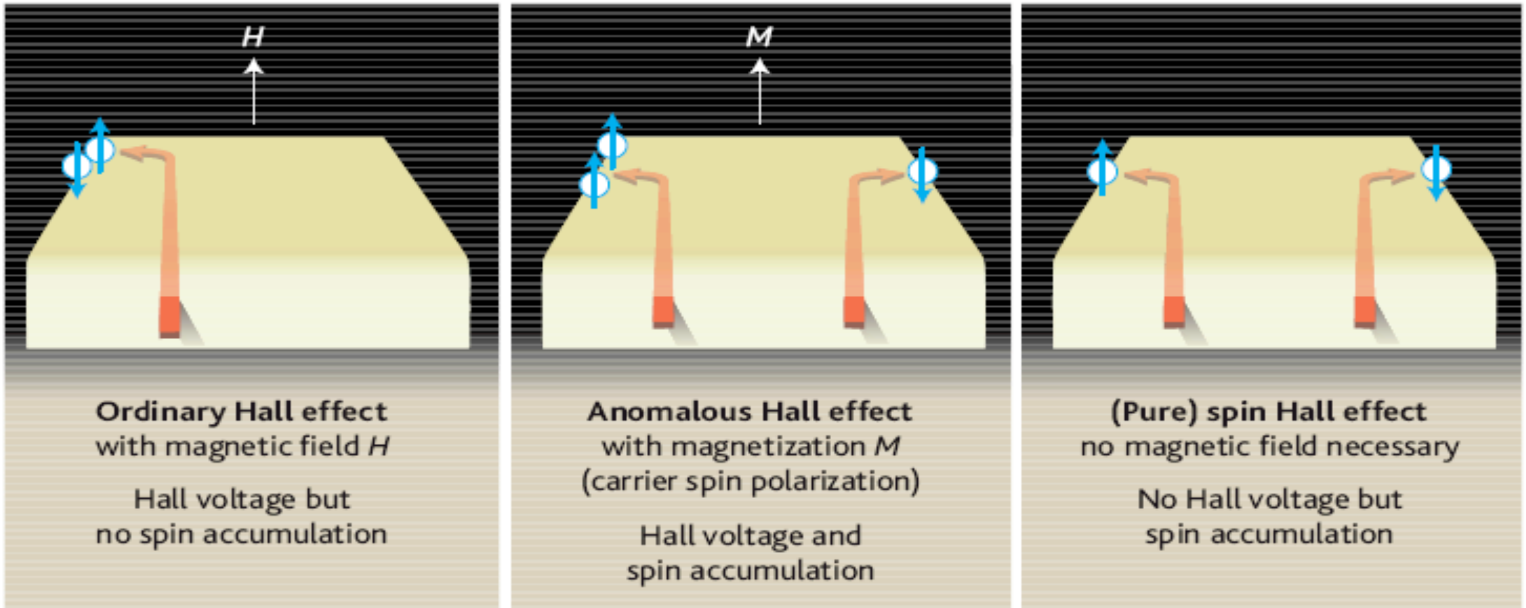
No net charge flow since the same number of electrons flow in each direction.

Since system has Fermi surface it dissipates, has longitudinal resistivity





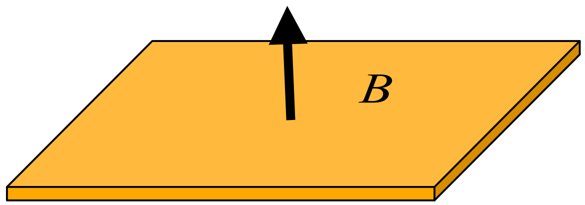




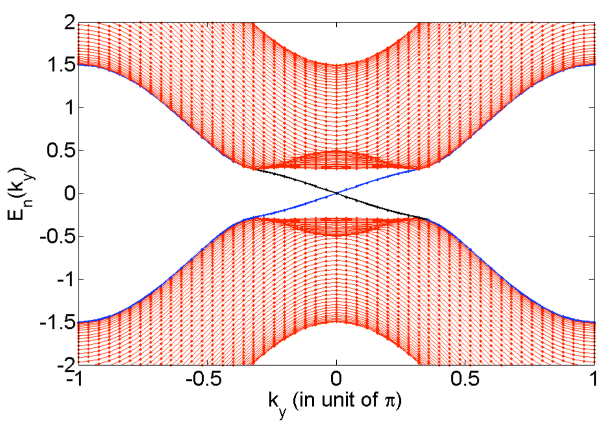
How about quantum spin Hall?

Quantum Hall Effect

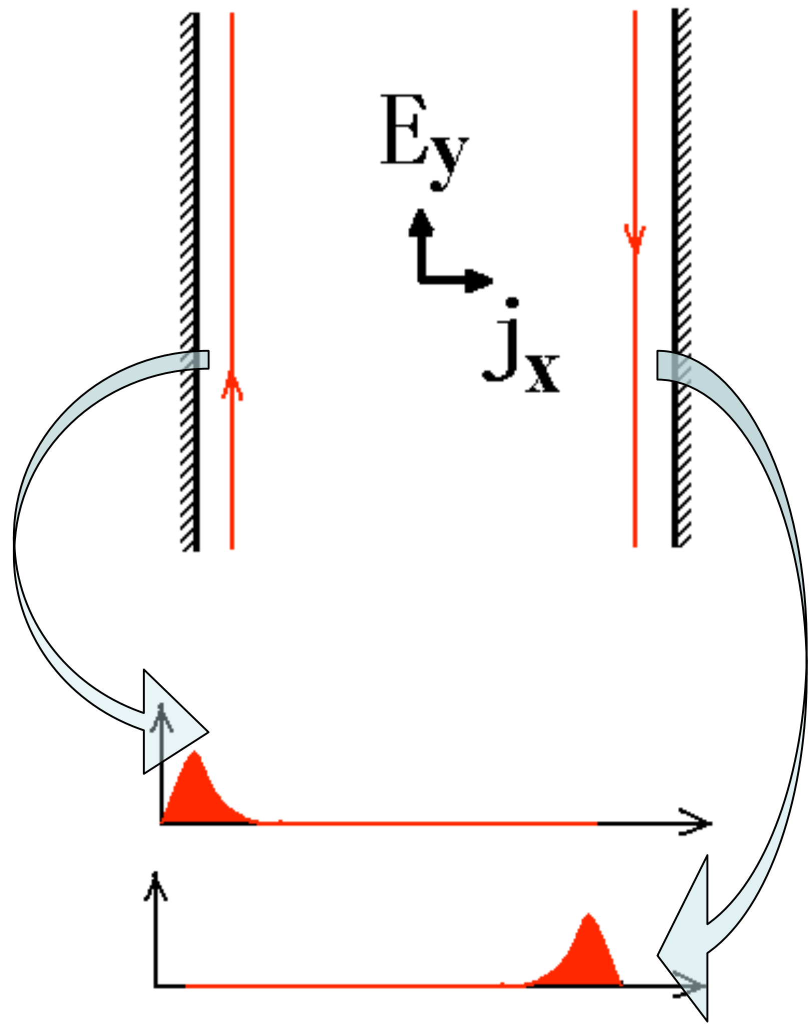
With Applied Magnetic Field



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



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



Dirac Fermion Revisited

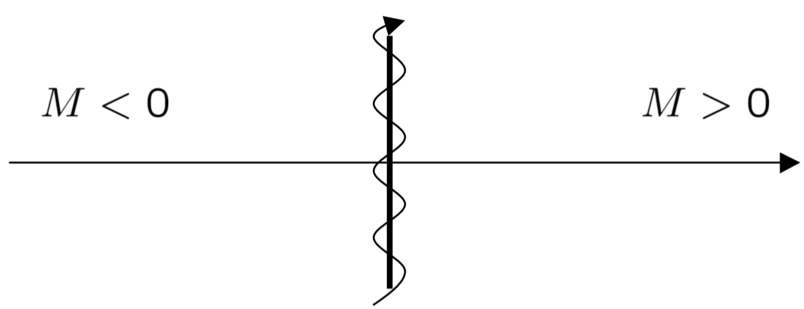
$$H = k_x\sigma_x + k_y\sigma_y + M\sigma_z$$

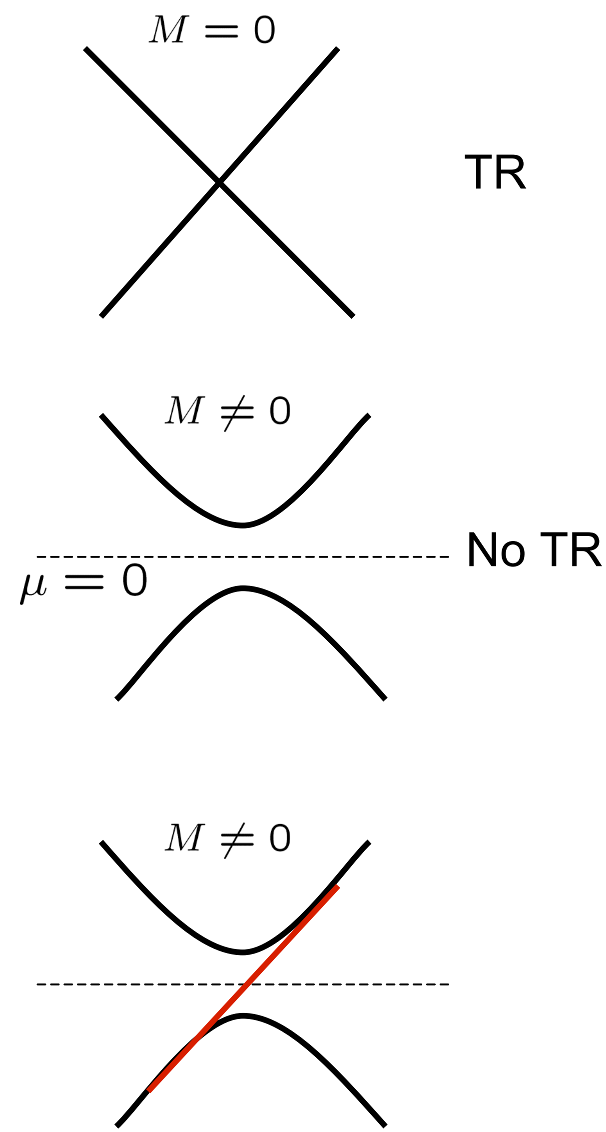
When gapped, a single Dirac fermion breaks time reversal

$$\sigma_{xy} = \lim_{\omega\to 0}\frac{1}{\omega}\langle J_x J_y\rangle(\omega) = \frac{1}{2}Sign(M)$$

Bulk-Edge correspondence

$$\sigma_{xy} = \frac{1}{2} - (-\frac{1}{2}) = 1$$

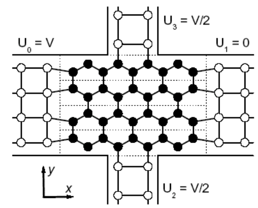




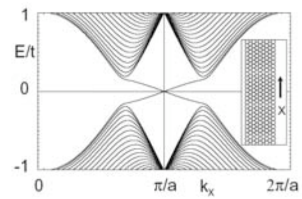
Quantum Spin Hall Effect

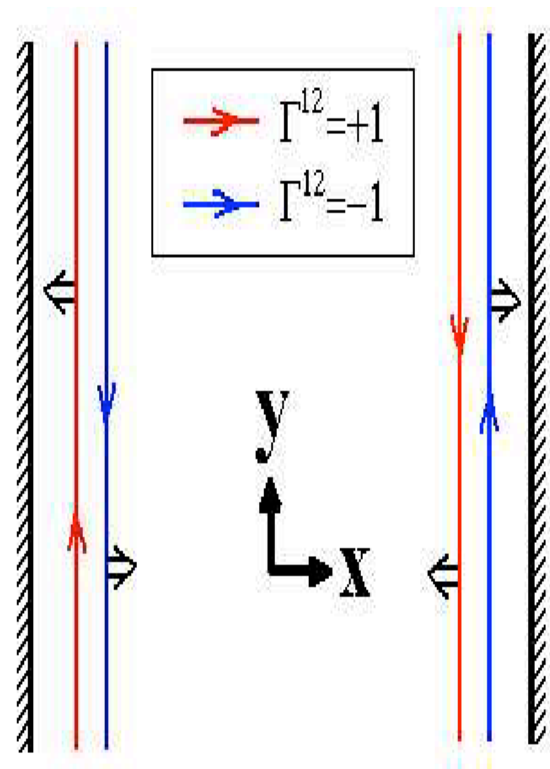
- Physical Understanding: Edge states

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



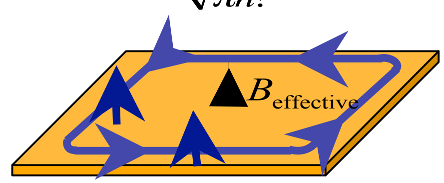
Graphene, Topological Semicond
by correlating the Haldane model with
spin (Kane and Mele, PRL (2005),
Qi, Wu, Zhang PRB (2006));



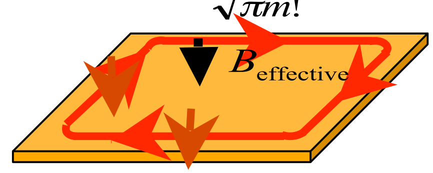


$$\phi_n = \frac{z^n}{\sqrt{\pi n!}} e^{-\frac{1}{2}zz^*}$$

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



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



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

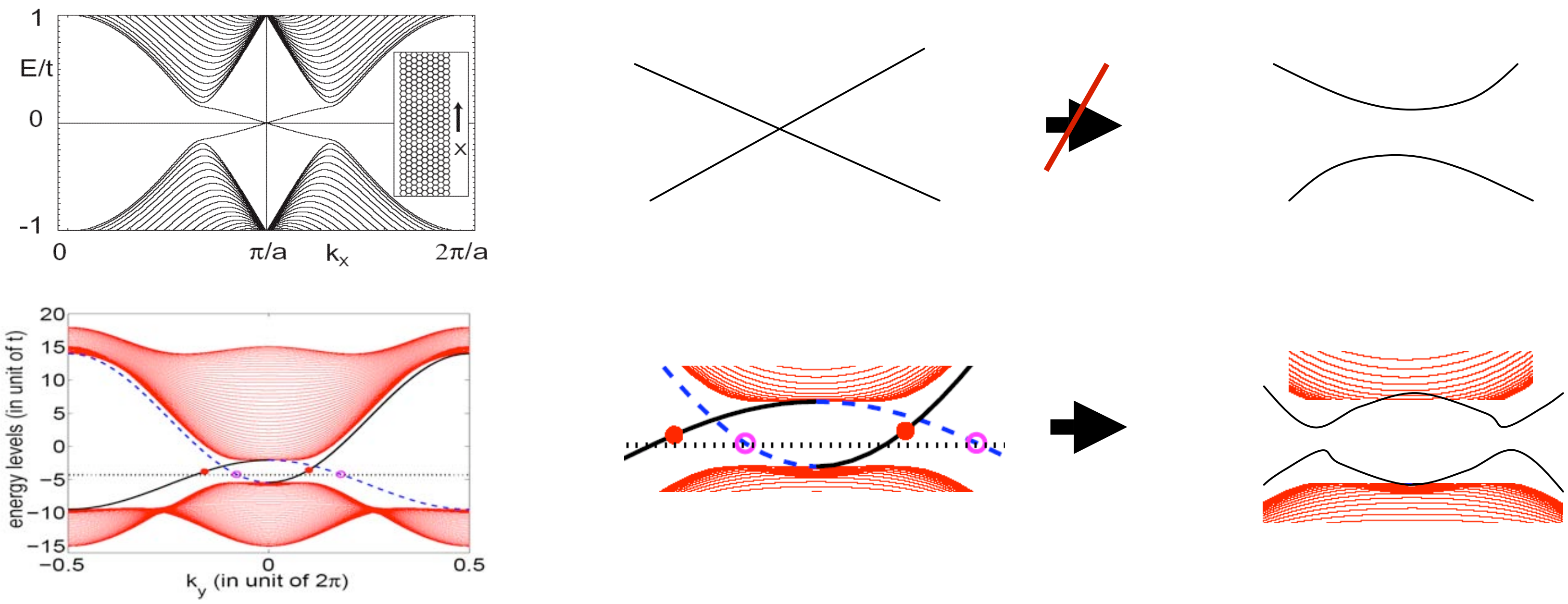
Z2 Topological classification

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

Kane and Mele PRL, (2005);

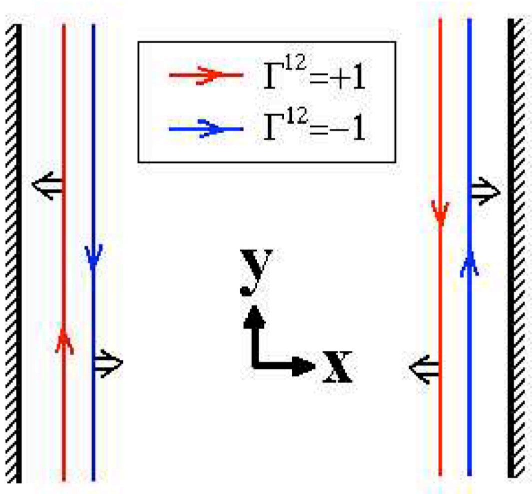
- Single particle backscattering not TR invariant – not allowed
- Umklapp relevant for K<½, opens gap for strong interactions.

Wu, Bernevig and Zhang PRL (2006), Xu and Moore, PRB (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.

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

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

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

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

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

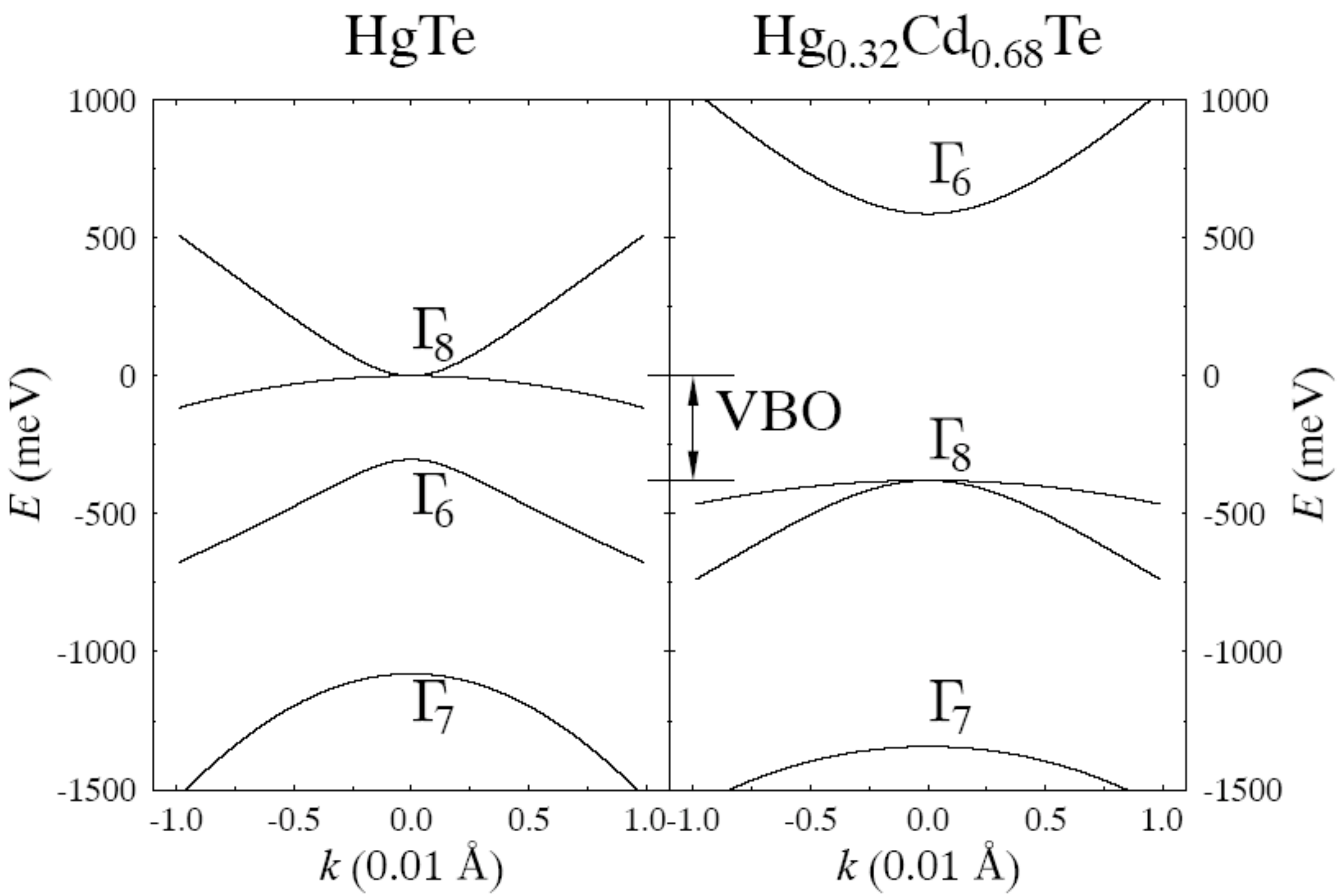
- A QSHE with even number of electron pairs for one edge is easy to open a TR invariant gap. For n=2 pairs:

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

Quantum Spin Hall Effect

- Goal: realistic proposal of the QSH state of matter in some material
- Do not require the knowledge of full topology of the bands
- Use only (controlled) pertubation theory

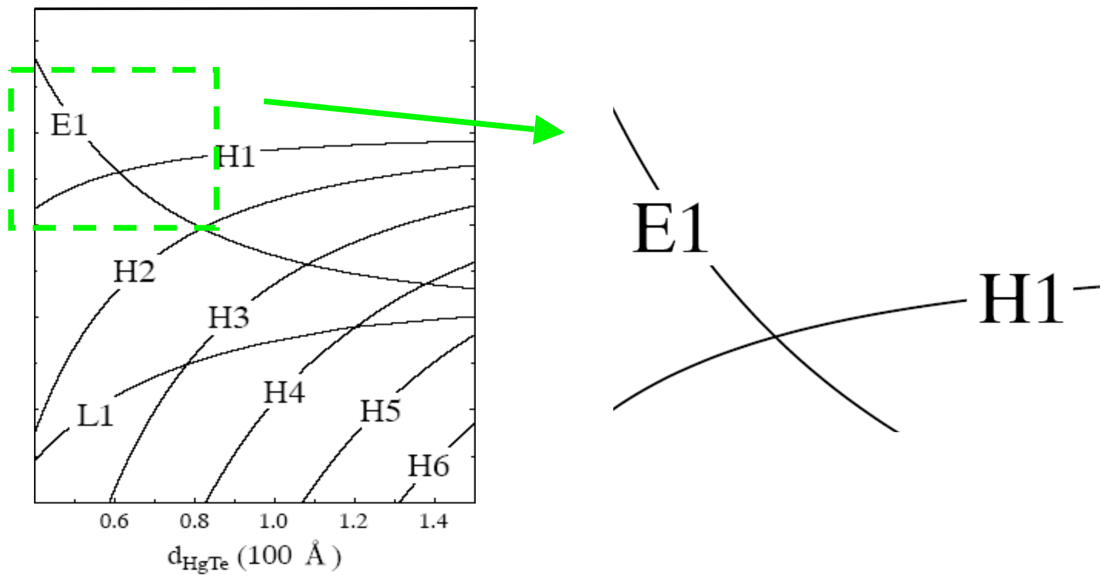
Bulk Band Structure

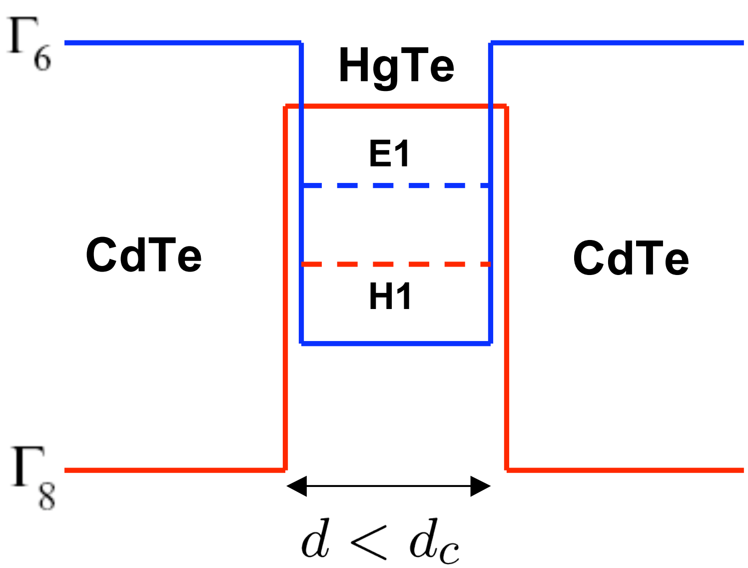


(see next talk)

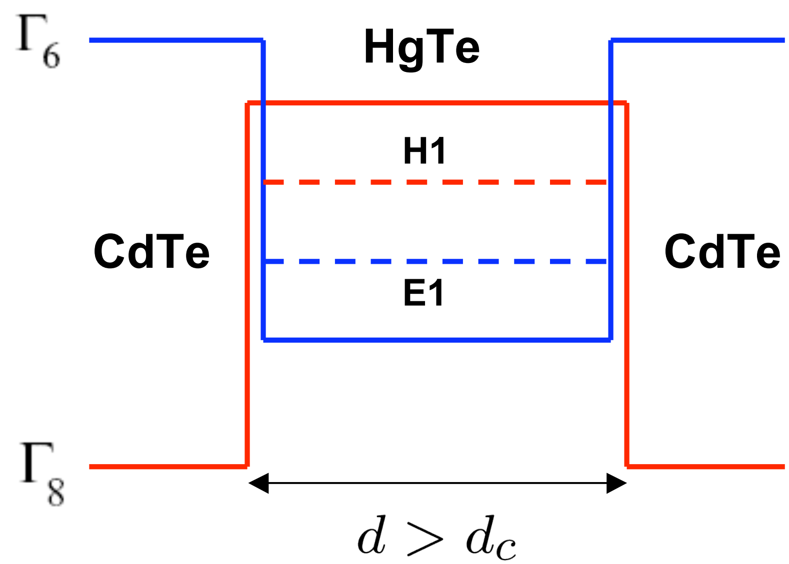
Quantum Well Sub-bands

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





normal



inverted

Envelope Functions

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

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

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

In $E1$, Γ_6 symm, Γ_8 antisymm $z- > -z$

Effective Hamiltonian E1, H1 bands close to crossing point

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

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

Effective 4-band Model

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

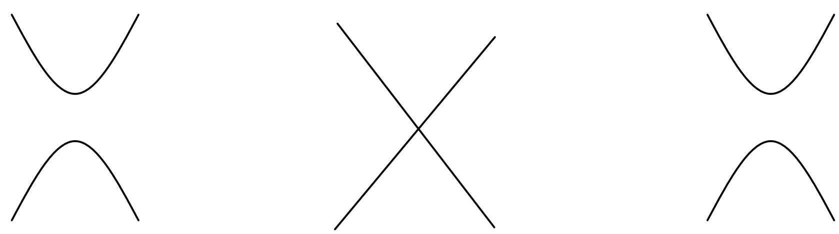
$$d_1 + i d_2 = A(k_x + i k_y) \equiv A k_+$$

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

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

Tunable graphene:



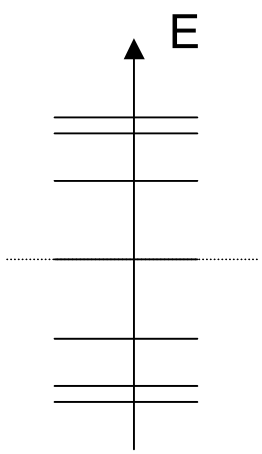
Continuum Picture

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:

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

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

For each block spin (they have opposite masses)

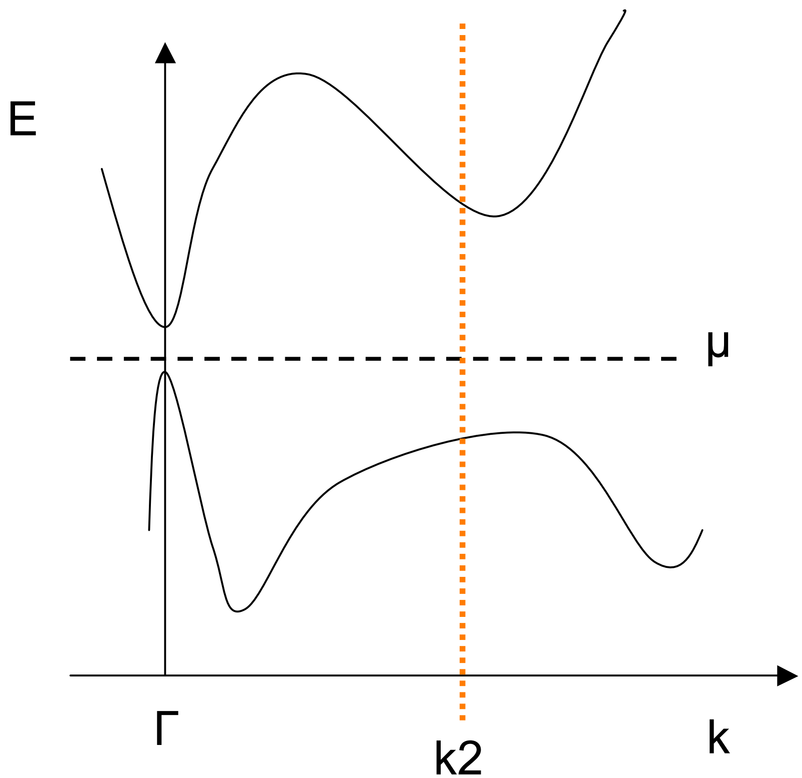


But this gives fractional quantum-Hall conductance for each block, so what is missing?

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 Γ point we get the contribution:

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

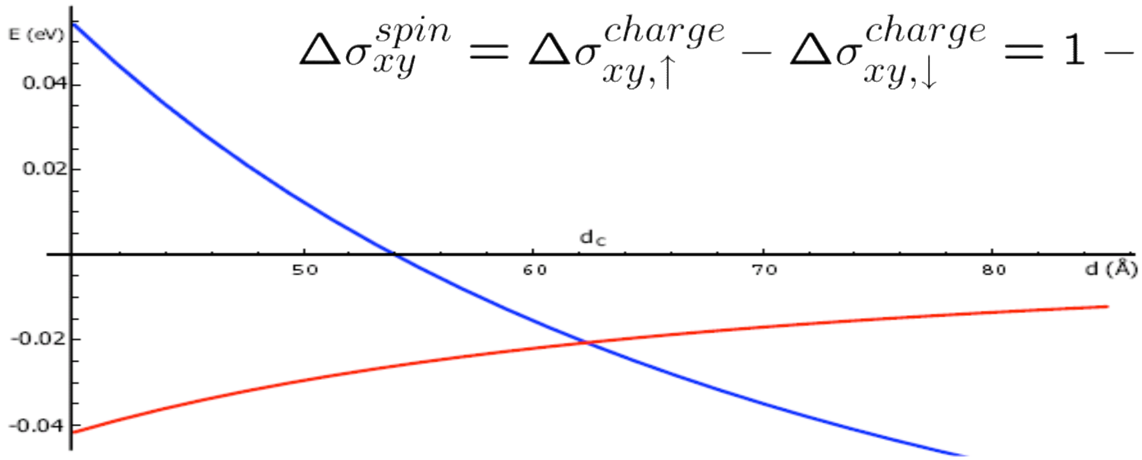
There is a "spectator fermion", generically in a higher energy part of BZ:

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

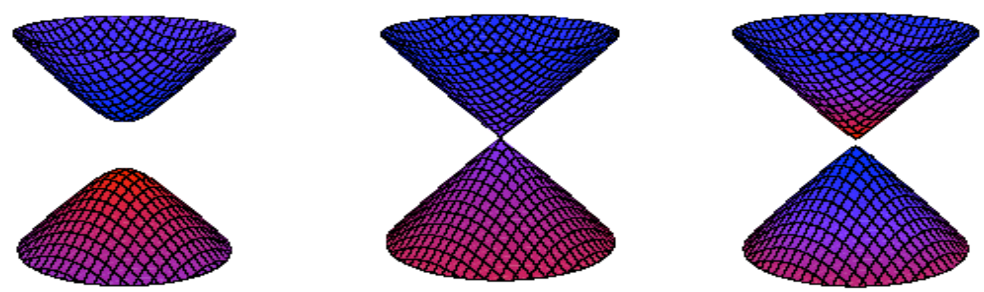
Does this add to the contribution at Γ or cancel it? Cannot know unless full BZ structure known, not only low-energy.

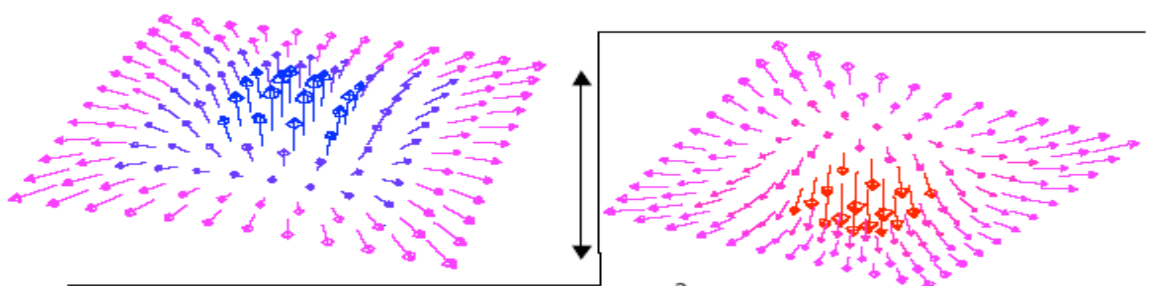
Physical Picture

$$\Delta\sigma_{xy}^{spin} = \Delta\sigma_{xy,\uparrow}^{charge} - \Delta\sigma_{xy,\downarrow}^{charge} = 1 - (-1) = 2$$



Meron in continuum picture:



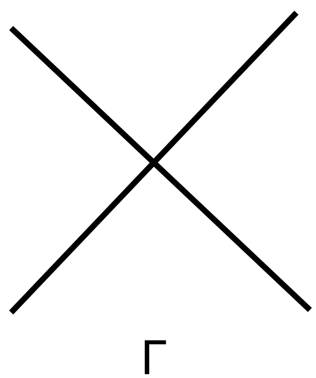


$$\Delta\sigma_{xy}^{(s)} = 2\frac{e^2}{h}$$

Change in Spin Hall Conductance

From k.p we cannot determine this since we only know about the Γ point

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



→ $\Delta\sigma_{xy}^{(s)} = \frac{2e^2}{h}$ (if we include both blocks)

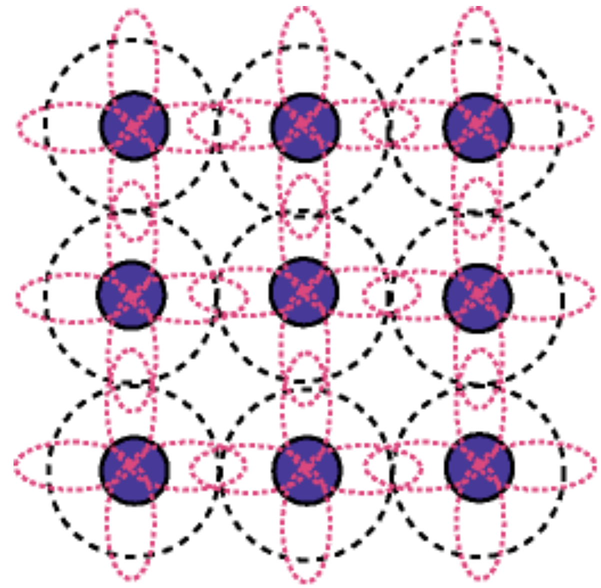
→ [Δ(# of pairs of edge states)] mod 2 =1 → QSHE exists on one side of transition

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.

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

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

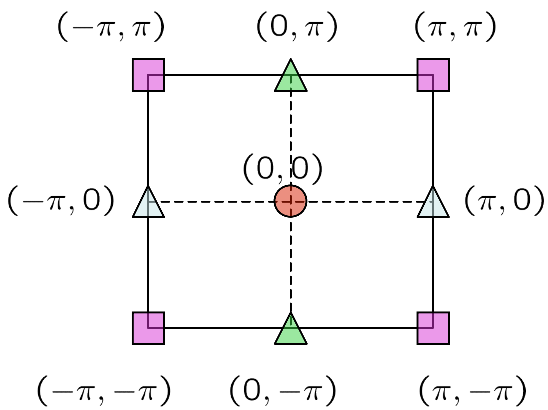
$$\mathcal{M}(k) = -2B(2 - \frac{M}{2B} - \cos(k_x) - \cos(k_y)),\ d_1 = A\sin(k_x),\ d_2 = A\sin(k_y), \text{ and } d_3 = \mathcal{M}(k)$$

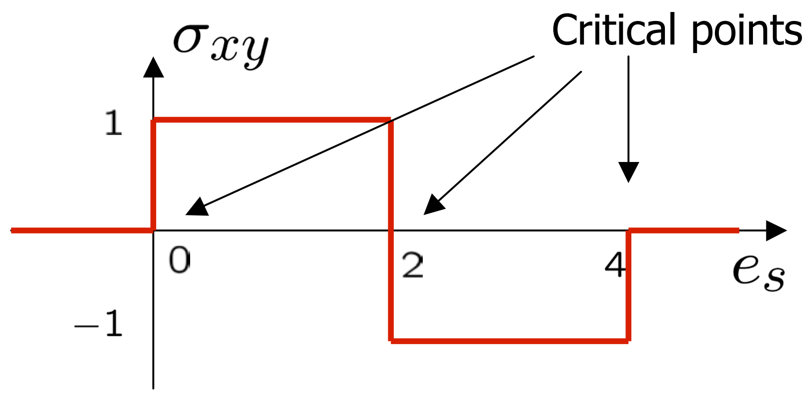
d (Å)	$A(eV)$	$B(eV)$	$C(eV)$	$D(eV)$	$M(eV)$
58	-3.62	-18.0	-0.0180	-0.594	0.00922
70	-3.42	-16.9	-0.0263	0.514	-0.00686

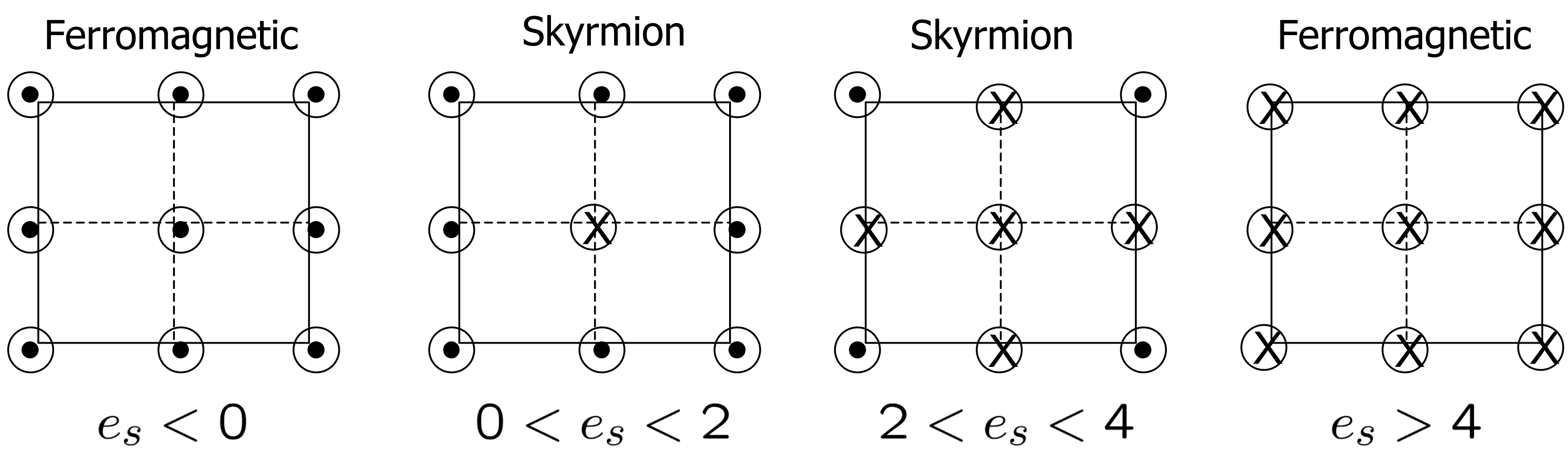
Topology of the tight-Binding Model

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

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

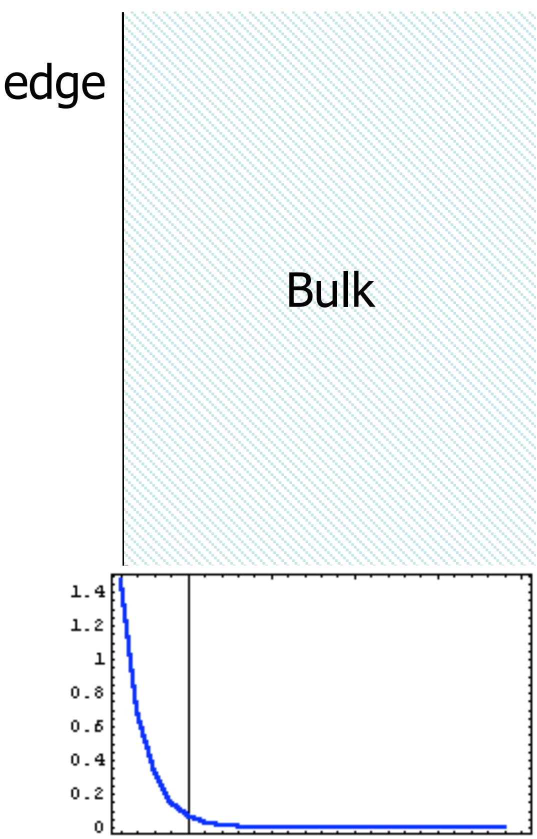


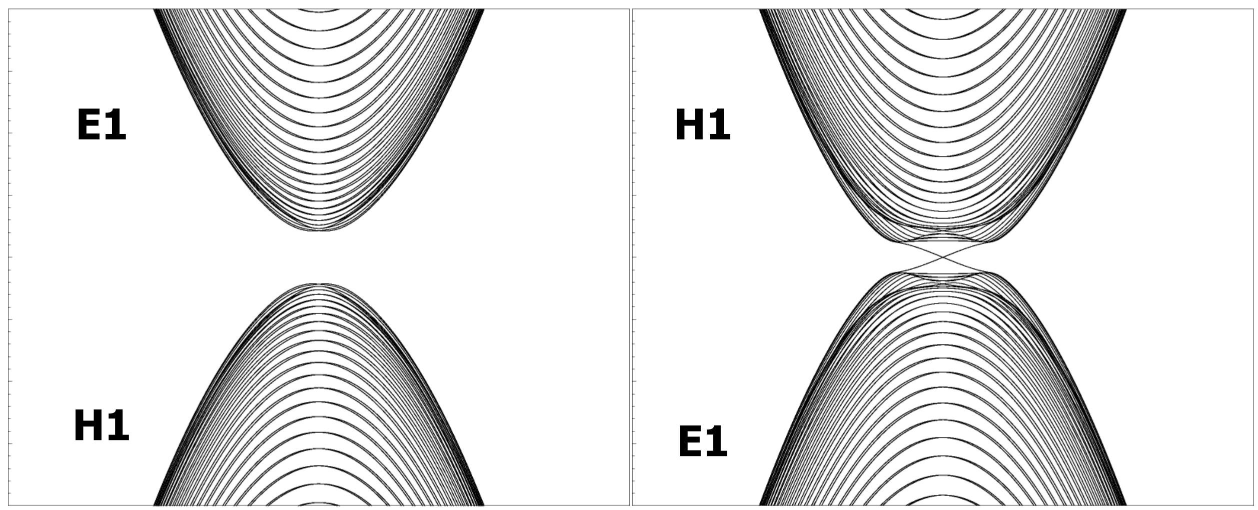




Edge states of the effective tight-binding model

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



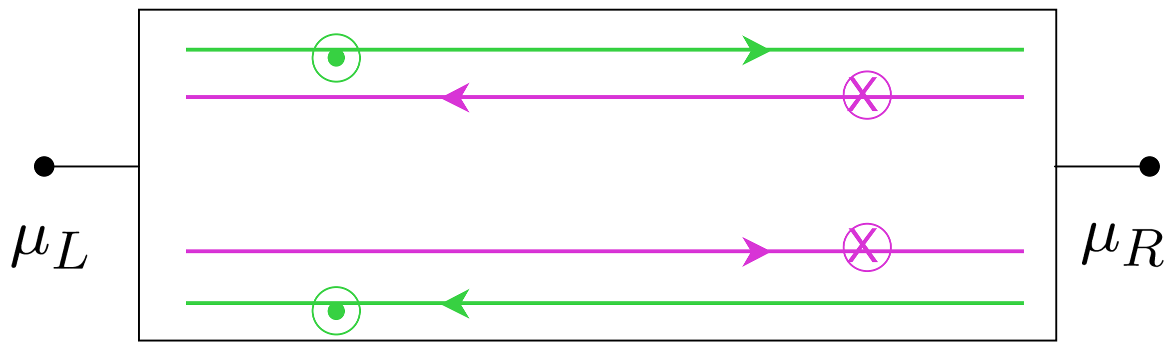


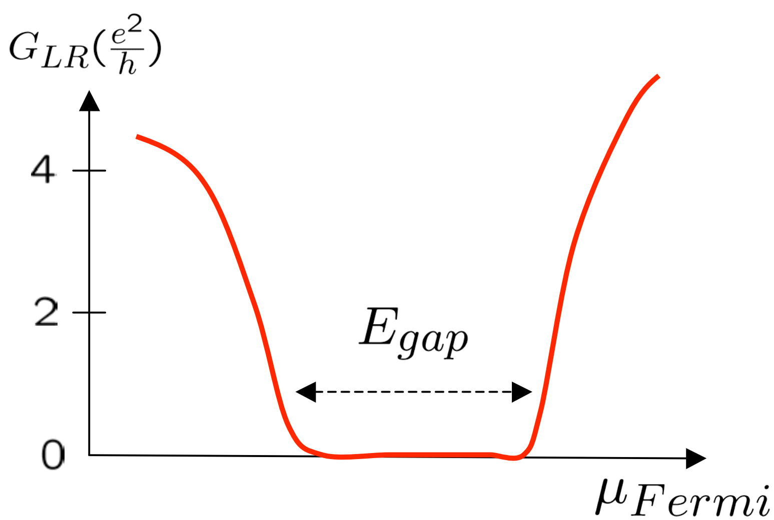
Trivial

Non-trivial

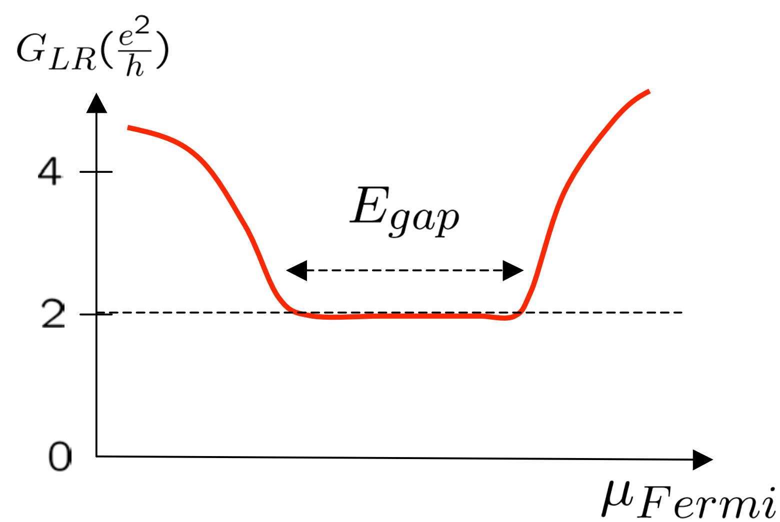
(neglecting kinetic energy term)

Experimental Signature (2-terminal)





$d < d_c$, normal regime



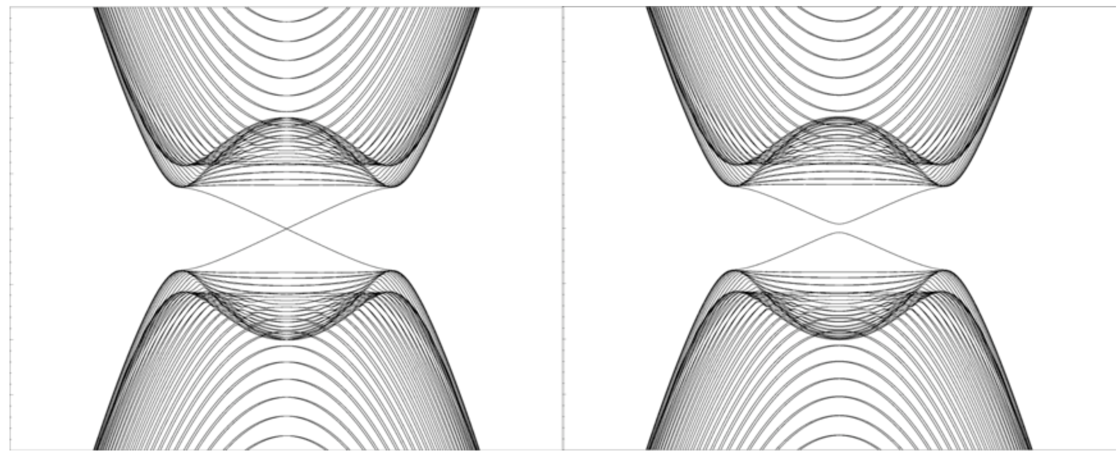
$d > d_c$, inverted regime

Smoking gun for the helical edge state: Magneto-Conductance

acknowledge conversations with C. Wu

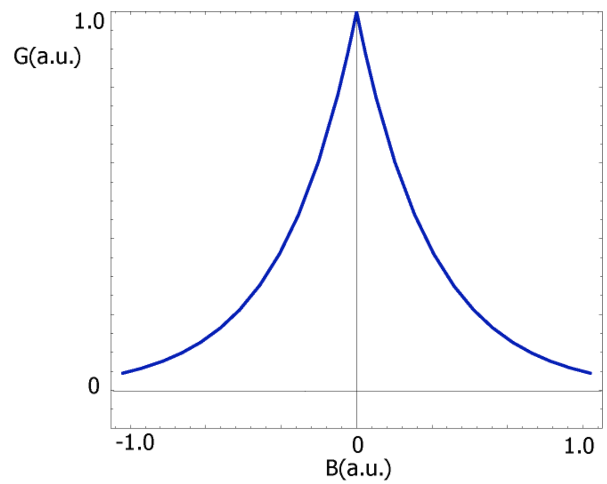
The crossing of the helical edge states is protected by the TR symmetry. TR breaking term such as the Zeeman magnetic field causes a singular perturbation and will open up a full insulating gap:

$$E_g \propto g|B|$$



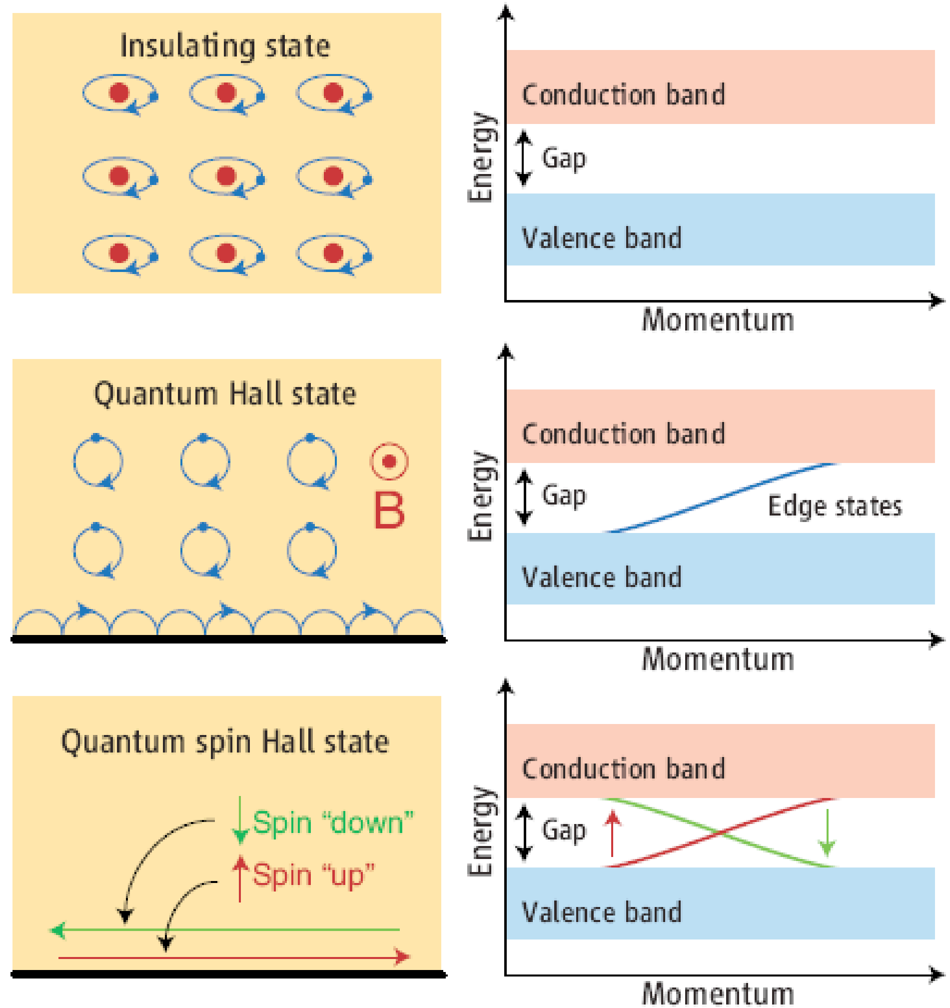
Conductance now takes the activated form:

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

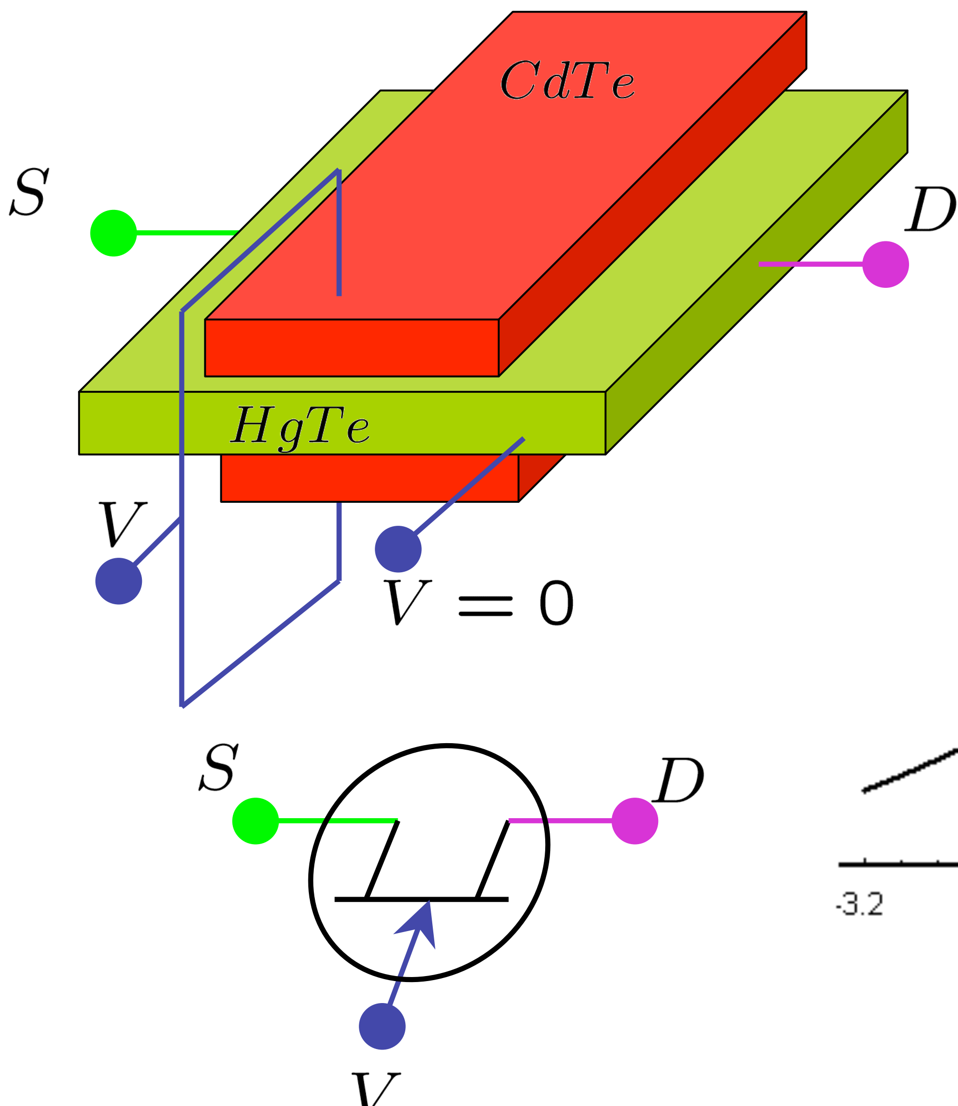


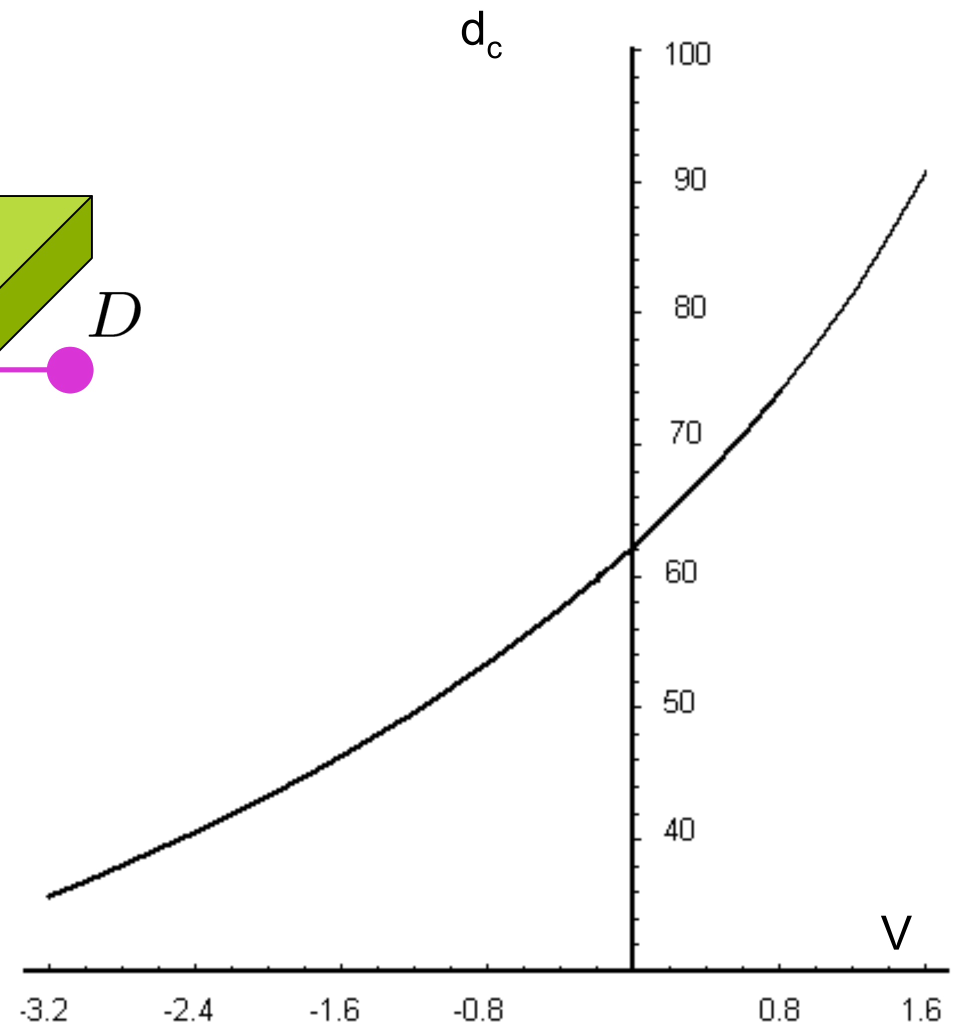
Conclusions

- 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.



QSHE Transistor

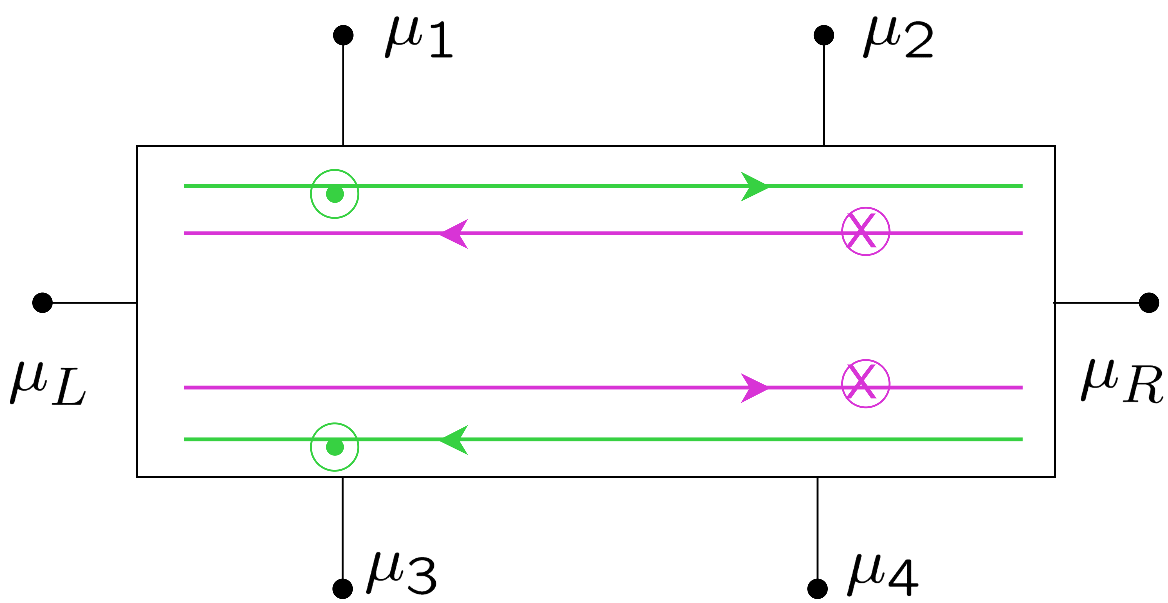




Conclusions

- QSHE and helical liquid
- QSHE state of matter must exist in HgTe quantum wells
- Lattice calculations indicate existence in “inverted” regime d>6 nm.
- Two clear experimental signatures
- Possibility to create transistor by relatively biasing CdTe and HgTe layers
- 3D topological insulators?

Experimental Signature (6-terminal)



A source-drain current j_LR ⟶ $\mu_1 = \mu_2$

$\mu_3 = \mu_4$

Chern Insulator in Magnetic Field

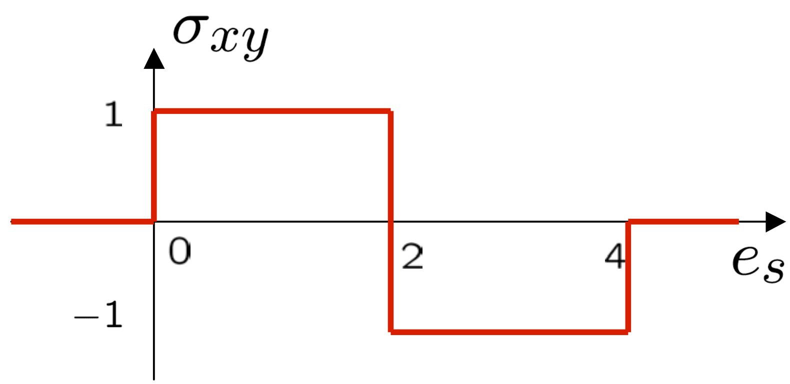
(acknowledge conversations with FDM Haldane)

- Interplay between the intrinsic Chern Insulator and the applied B field Landau Physics
- Valid for magnetic semiconductors with Quantum Anomalous Hall effect
- Also valid for Quantum Spin Hall effect in fully polarized limit

$$\mathcal{H} = d_i(\vec{k})\sigma_i$$

$$d_1 = A \sin k_x, \quad d_2 = A \sin k_y,$$

$$d_3 = 2 - M - \cos kx - \cos ky$$

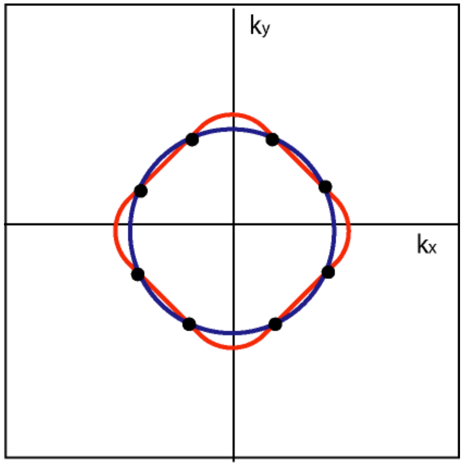


•Add B of flux p/q $\quad \exp(i \int \vec{A} d\vec{r}) \quad \vec{A} = (-By, 0, 0) \quad B = \frac{p}{q}(\frac{\Phi_0}{a^2})$

Inversion symmetry breaking in zincblend lattices

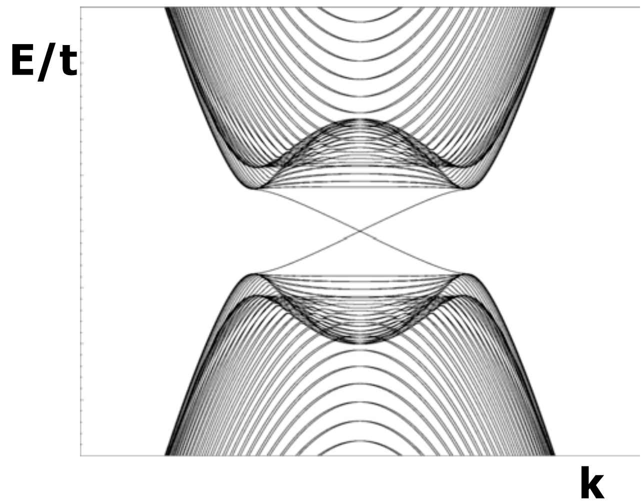
Inversion breaking term comes in the form:

$$C(< k_z > + \ldots)\{J_z, J_x^2 - J_y^2\},$$ $J_x,\ J_y,\ J_z$ -spin 3/2 matrices



which couples E1+, H1- and E1-,H1+ states and is a constant in quasi-2d systems

$$H_{\Delta}^{eff} = \begin{pmatrix} 0 & 0 & 0 & -\Delta \\ 0 & 0 & \Delta & 0 \\ 0 & \Delta & 0 & 0 \\ -\Delta & 0 & 0 & 0 \end{pmatrix}$$



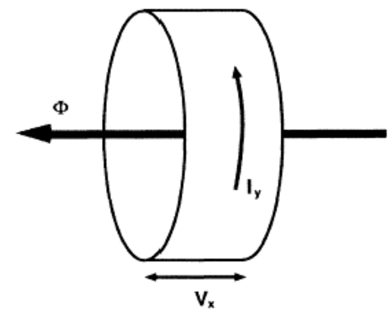
Gap closes at nodes away from k=0, gap reopens at non-zero value of M/2B.
In the inverted regime, the helical edge state crossing is still robust.

Hatsugai Method

$$H = -t_x \sum_{m,n} c^\dagger_{m+1,n} c_{m,n}$$
$$-t_y e^{i\frac{2\pi\Phi}{L_y}} \sum_{m,n} c^\dagger_{m,n+1} e^{i2\pi\phi m} c_{m,n} + \text{H.c.},$$

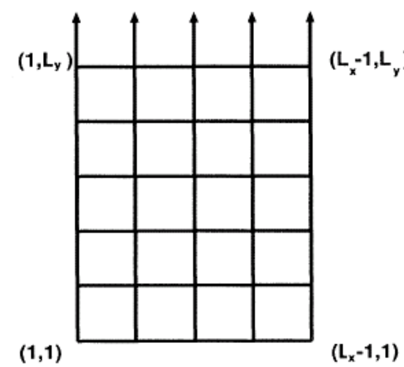
$$-t_x\{\Psi_{m+1}(k_y,\Phi) + \Psi_{m-1}(k_y,\Phi)\}$$
$$-2t_y \cos\left(k_y - 2\pi\frac{\Phi}{L_y} - 2\pi\phi m\right)\Psi_m(k_y,\Phi) = E\Psi_m(k_y,\Phi)$$

$$\begin{pmatrix} \Psi_{m+1}(\epsilon,k_y,\Phi) \\ \Psi_m(\epsilon,k_y,\Phi) \end{pmatrix} = \tilde{M}_m(\epsilon,k_y,\Phi) \begin{pmatrix} \Psi_m(\epsilon,k_y,\Phi) \\ \Psi_{m-1}(\epsilon,k_y,\Phi) \end{pmatrix}$$



TM over magnetic unit cell (2 \times 2)

$$M(\epsilon) = \begin{pmatrix} M_{11}(\epsilon) & M_{12}(\epsilon) \\ M_{21}(\epsilon) & M_{22}(\epsilon) \end{pmatrix} \equiv \tilde{M}_q \tilde{M}_{q-1} \ldots \tilde{M}_1.$$



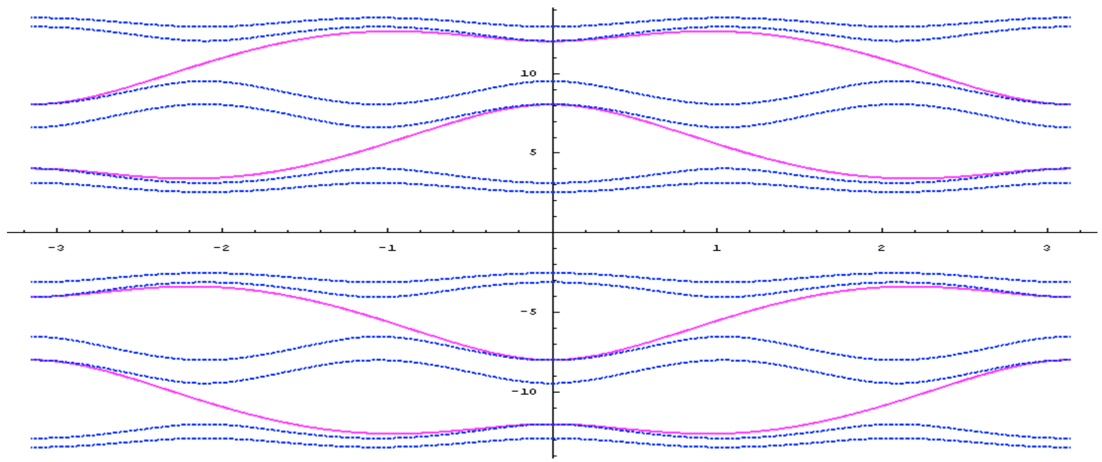
For each k, the elements of the matrix are polynomials energy

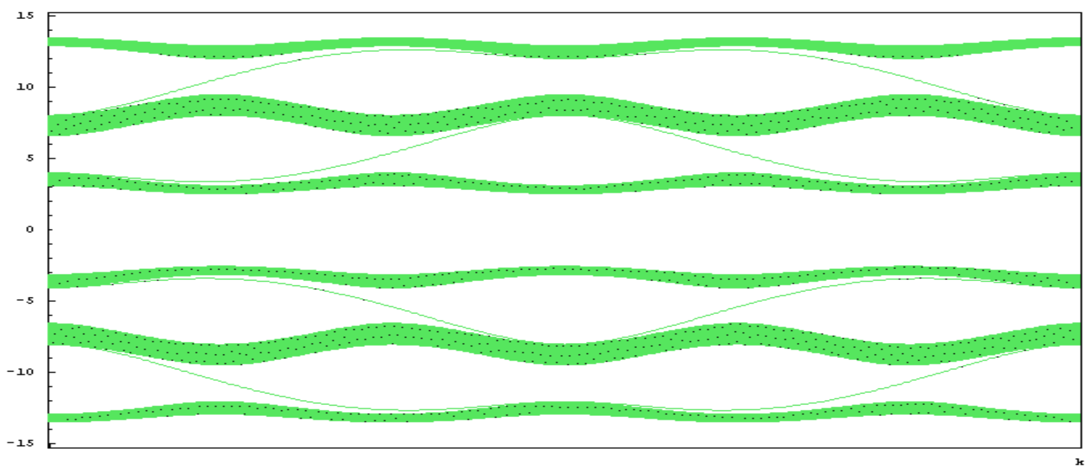
Edge states $M_{21}(\epsilon) = 0$

Bands $(Tr[M])^2 = 4$

Hatsugai Method

q=3





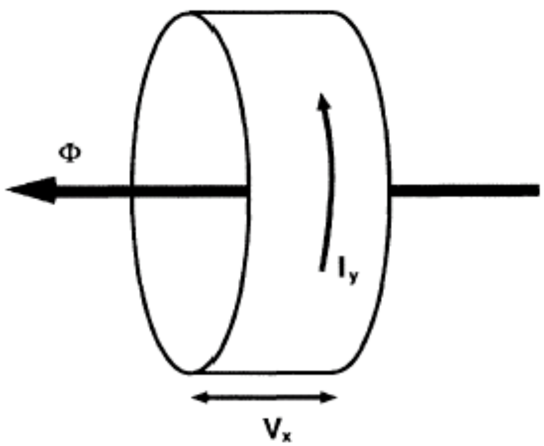
Brought to you by PITP (www.pitp.phas.ubc.ca)

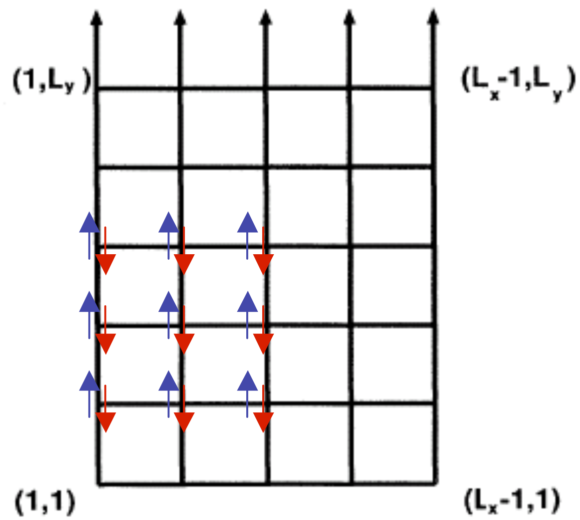
Generalization of Hatsugai Method

Generalization of Harper Equation to matrix Hamiltonian

$$\begin{pmatrix} \Psi_{m+1,\uparrow} \\ \Psi_{m+1,\downarrow} \\ \Psi_{m,\uparrow} \\ \Psi_{m,\downarrow} \end{pmatrix} = \hat{M}(m) \begin{pmatrix} \Psi_{m,\uparrow} \\ \Psi_{m,\downarrow} \\ \Psi_{m-1,\uparrow} \\ \Psi_{m-1,\downarrow} \end{pmatrix}$$

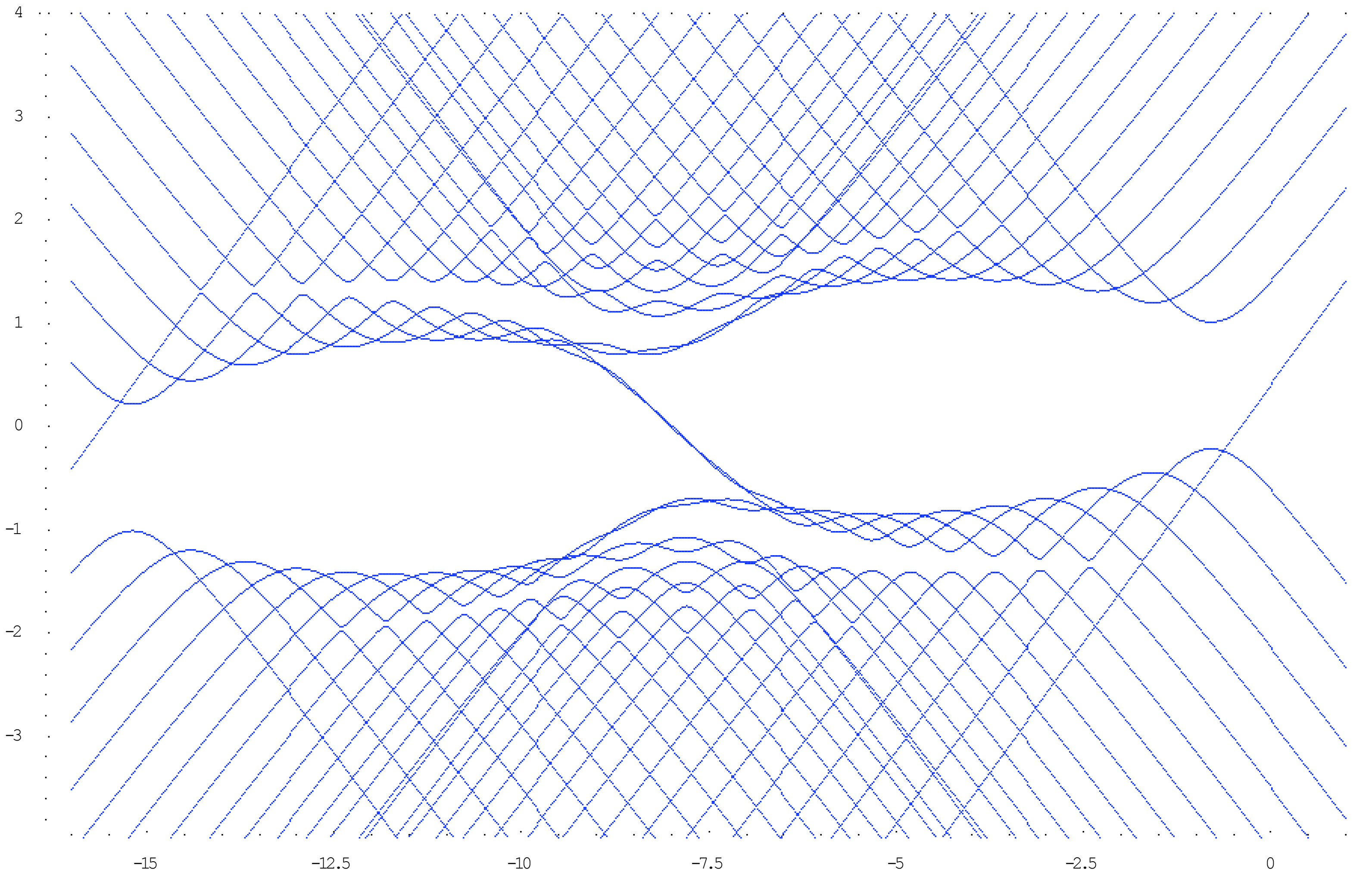
$$M = \hat{M}(q) \ldots \hat{M}(1)$$





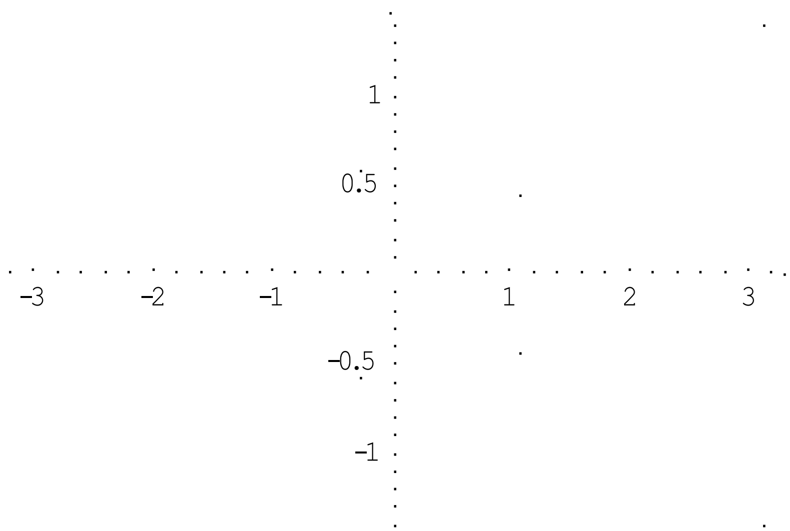
Hamiltonian Spectrum: Exact Lattice Results

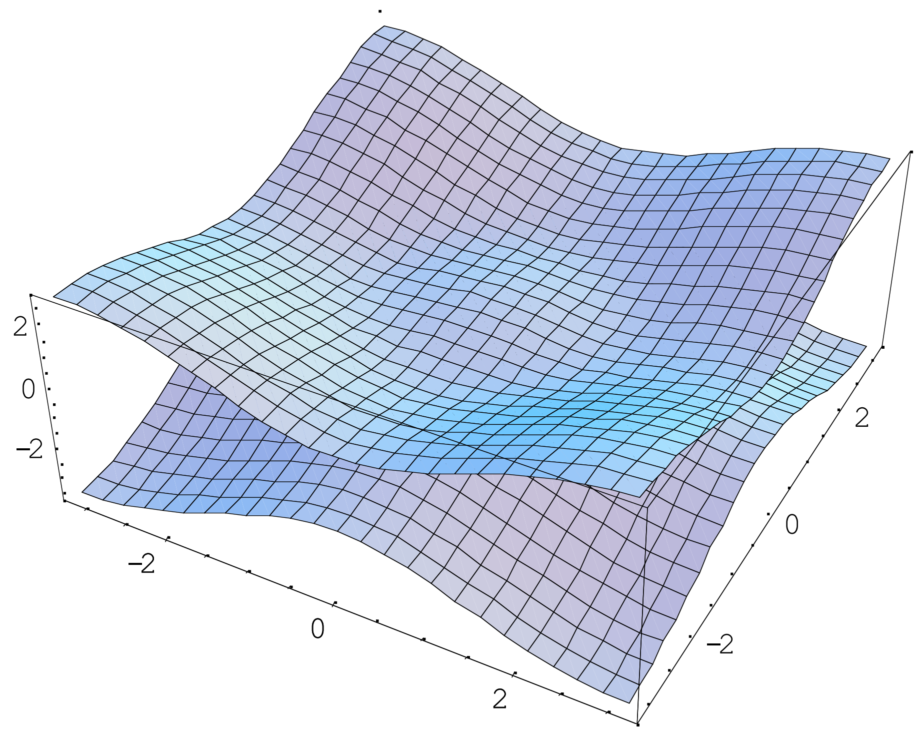
q=30

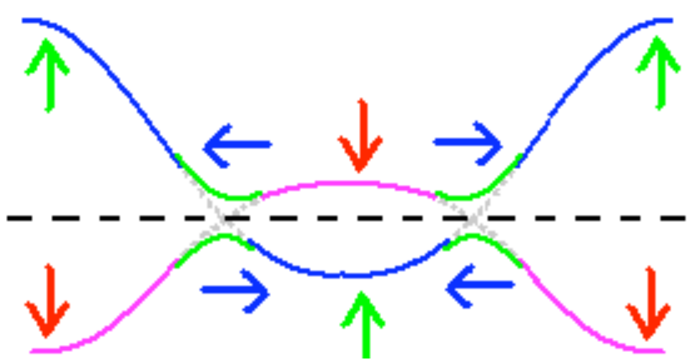


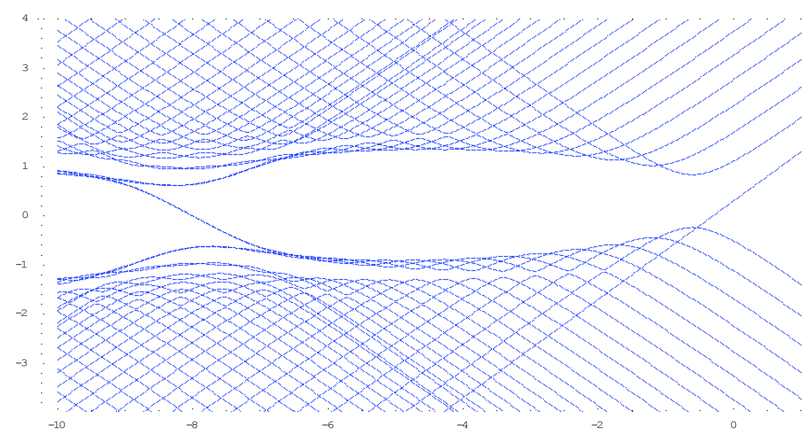
$M = -4$ $M = -2$ $M = 0$

Hamiltonian Spectrum



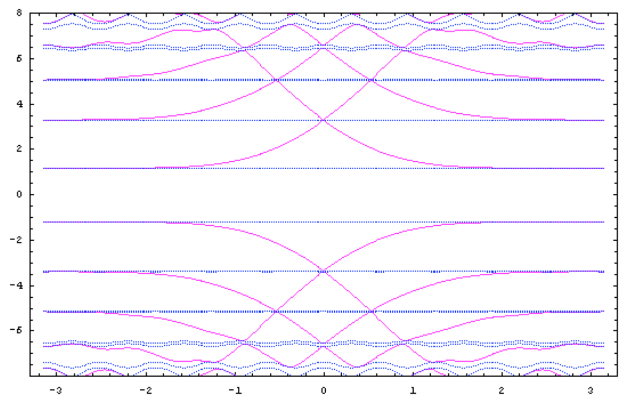


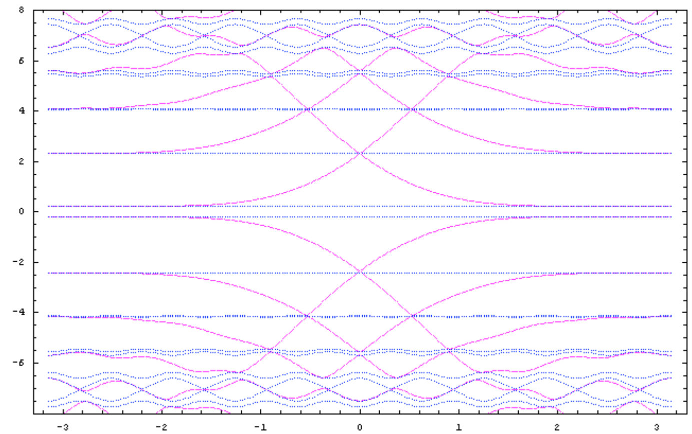


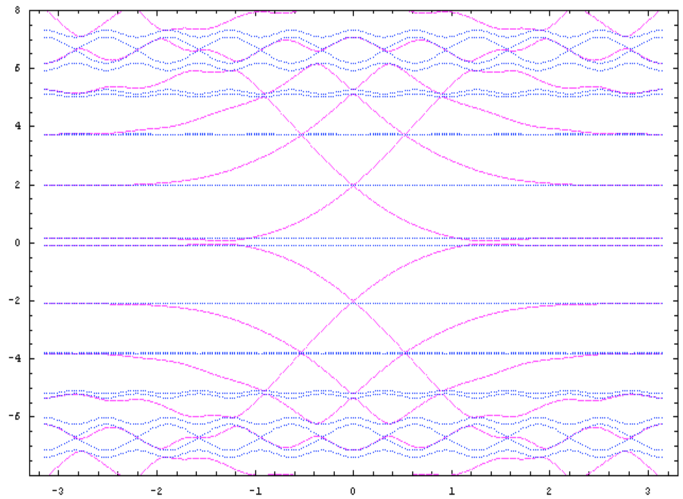


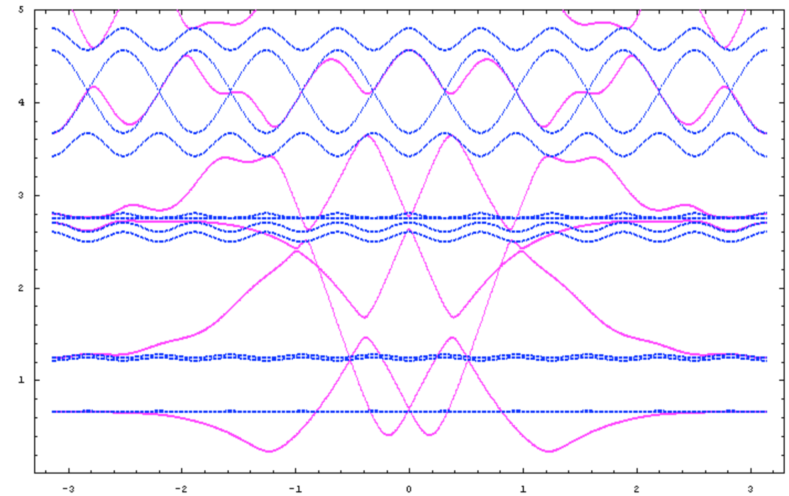
Edge State Spectrum

q=10, increasing gap, thru the chern insulator transition









Quantum Anomalous Hall Effect

Qi et al, 2006

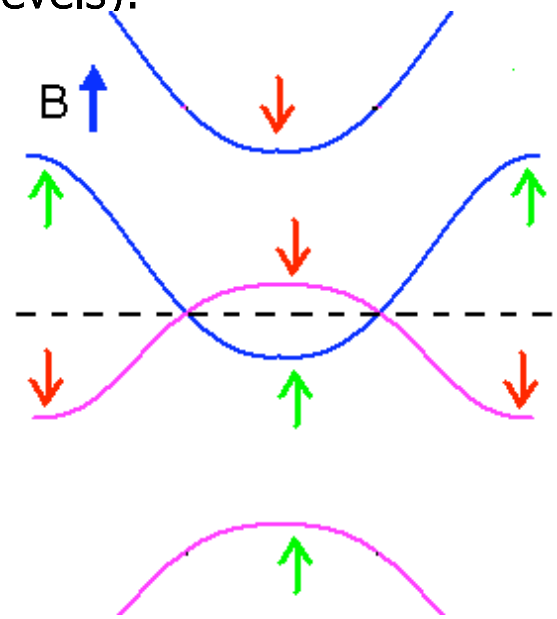
Magnetic semiconductor with SO coupling (no Landau levels):

General 2×2 Hamiltonian

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

Example

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

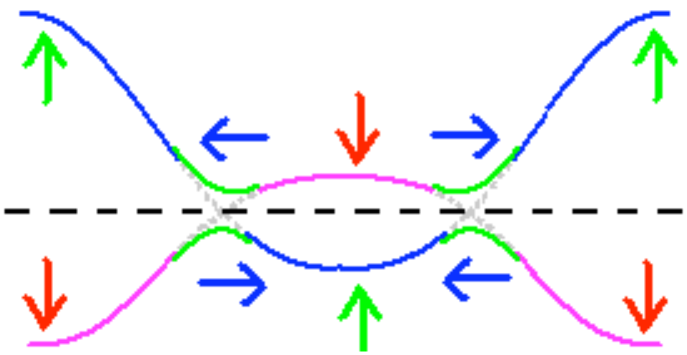


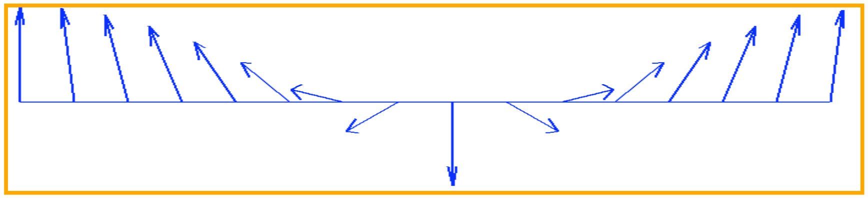
Quantum Anomalous Hall Effect

Hall Conductivity

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

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





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<½

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

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

- 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:

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