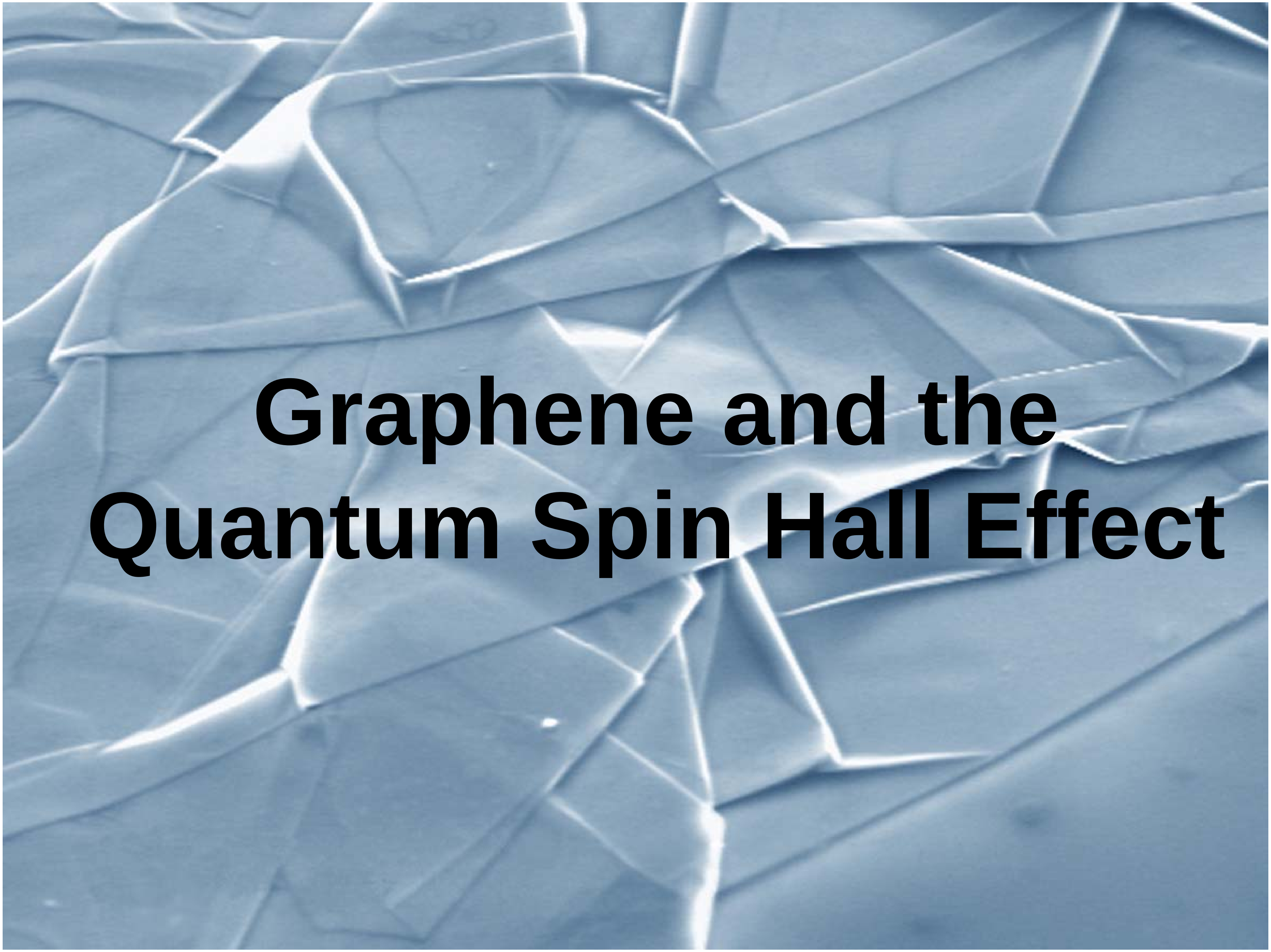
Graphene and the Quantum Spin Hall Effect



Graphene, the Quantum Spin Hall Effect and topological insulators

I. Graphene

II. Quantum Spin Hall Effect

- Spin orbit induced energy gap in graphene
  - $\Rightarrow$ A new 2D electronic phase
- Gapless Edge states and transport
- Time Reversal symmetry and Z_2 topological stability.

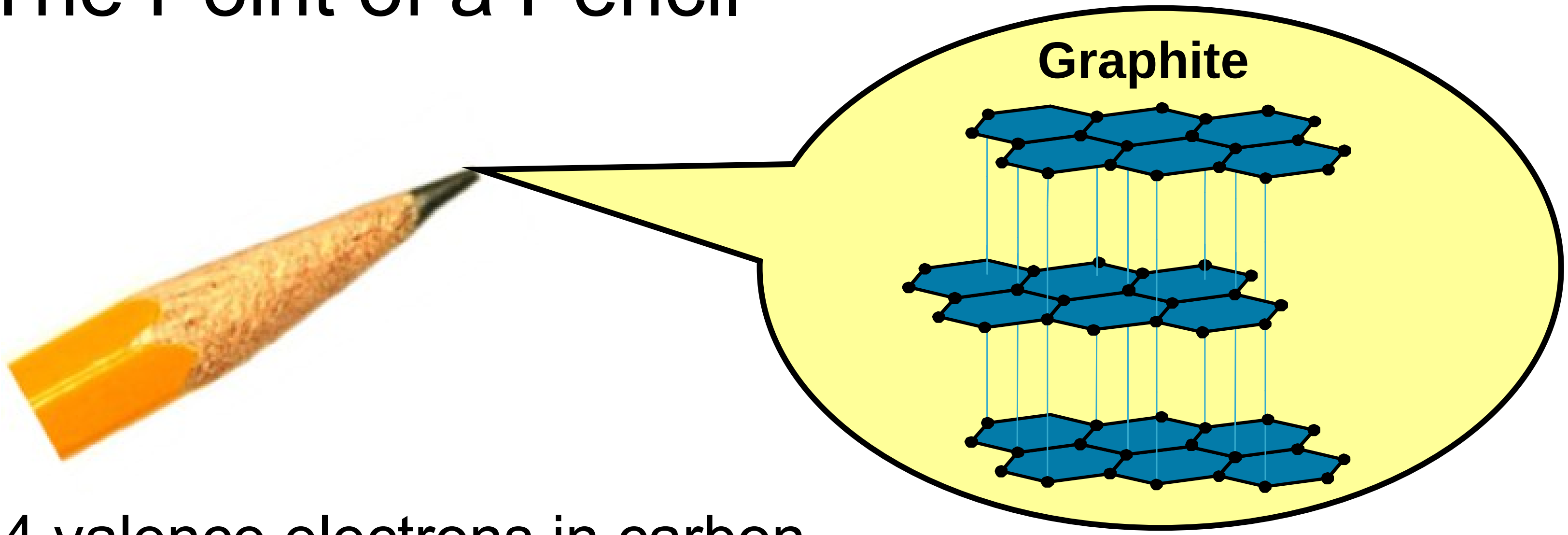
III. Three Dimensional Generalization

- Topological Insulator, Surface States
- Specific Materials

CL Kane & EJ Mele, PRL 95, 226801 (05); PRL 95 146802 (05).
L Fu & CL Kane, PRB 74, 195312 (06), cond-mat/0611341
L Fu, CL Kane & EJ Mele, PRL 98, 106803 (07)

Thanks to Gene Mele, Liang Fu

The Point of a Pencil



4 valence electrons in carbon

- 3 bonds to neighbors (sp^2 σ bonds)

    Structural Rigidity within planes

    Weak Van der Waals attraction between planes

- 1 delocalized π electron

    Electrical Conductivity

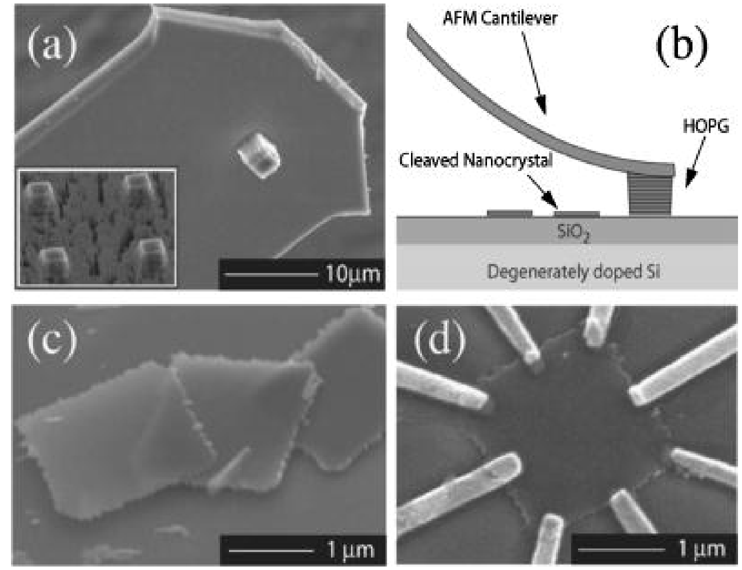
Graphene = A single layer of graphite

A unique 2D electronic material

Isolating Single Planes of Graphene

Philip Kim (Columbia)
Zhang et al. APL 2004

"Nanopencil" on AFM cantilever deposits ~ 15 layer graphite films



Andre Geim (Manchester)
Novoselov et al. Science 2004

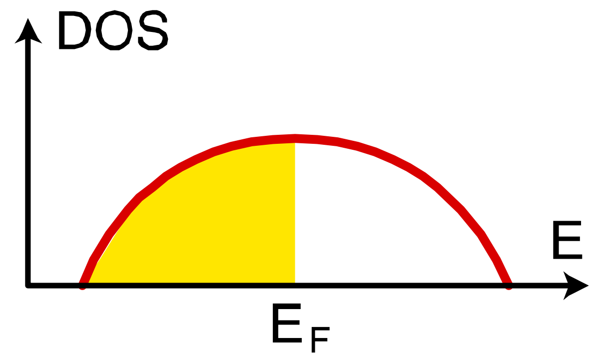
Individual layers on SiO_2 prepared by mechanical exfoliation.

SEM

Electronic Structure

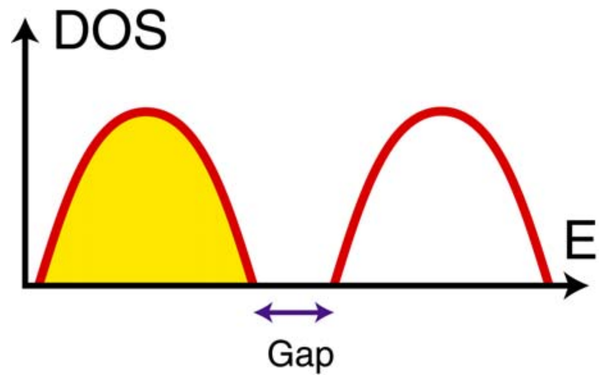
Metal

- Partially filled band
- Finite Density of States (DOS) at Fermi Energy



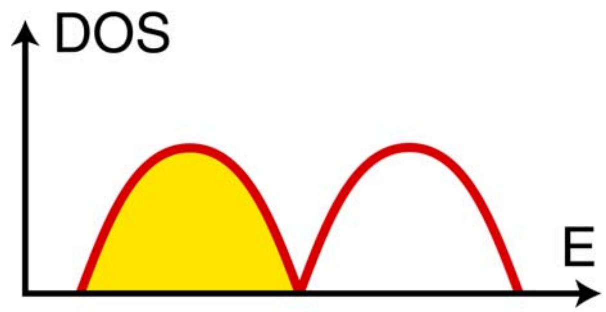
Semiconductor

- Filled Band
- Gap at Fermi Energy

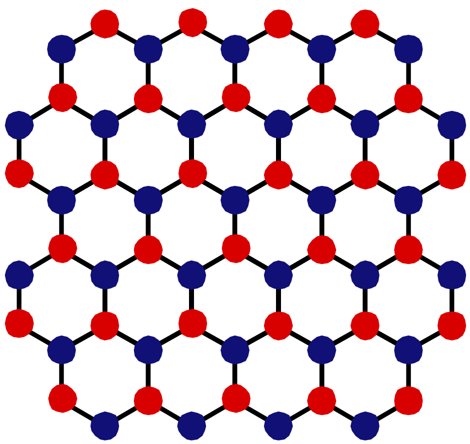


Graphene A critical state

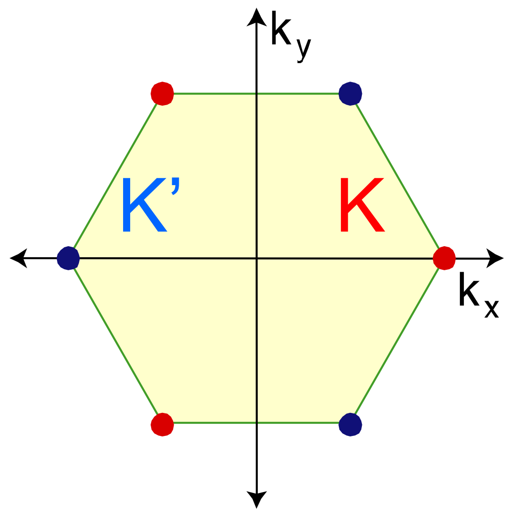
- Zero Gap Semiconductor
- Zero DOS metal



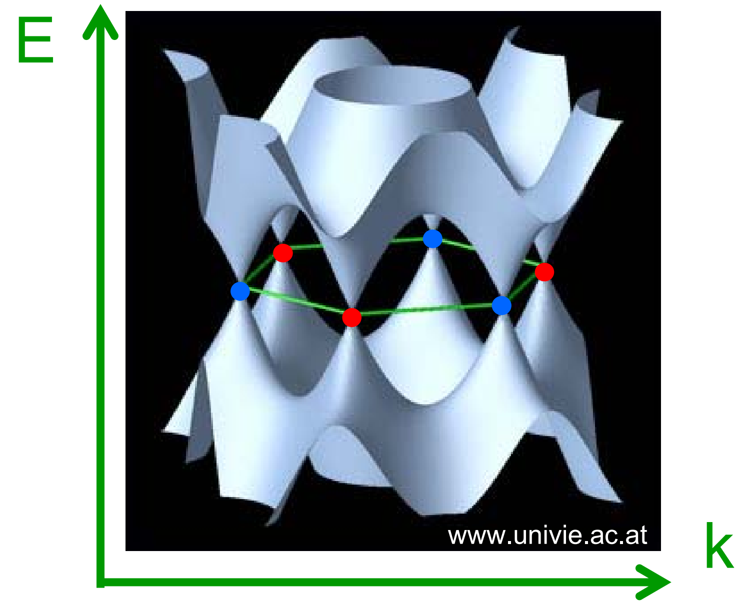
Tight Binding Model for π electrons on honeycomb lattice



Honeycomb Lattice



Brillouin Zone



- The conduction band and valence band touch at two "Fermi points" K and K'.
- Near K and K' the dispersion is "*relativistic*" (ie linear).

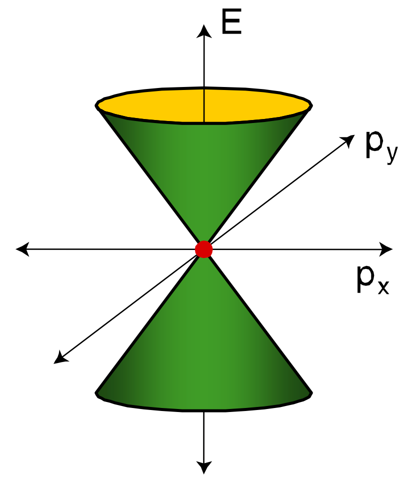
$$E(\mathrm{K}+\vec{q}) = \pm\hbar v_F \,|\, \vec{q} \,|$$

"Metallic" Fermi velocity
$v_F \sim 7 \times 10^5$ m/s ~ c/400

Low Energy Theory: Effective Mass (or k•p) model

DiVincenzo, Mele (84)

(Exact Wavefunction) = (Wavefunction at K or K') × ($\psi(x)$: Slow Modulation)



- Massless Dirac Fermions in 2+1 Dimensions

$$H_{eff}\psi = i\hbar v_F (\vec{\Gamma}\cdot\vec{\nabla})\psi$$

- 8 components :

$$\psi = \psi_{a\alpha s}$$

a =	A or B	Sublattice index	$\sigma^z_{ab'}$
α =	K or K'	K point index	$\tau^z_{\alpha\alpha'}$
s =	↑ or ↓	Spin index	$s^z_{ss'}$

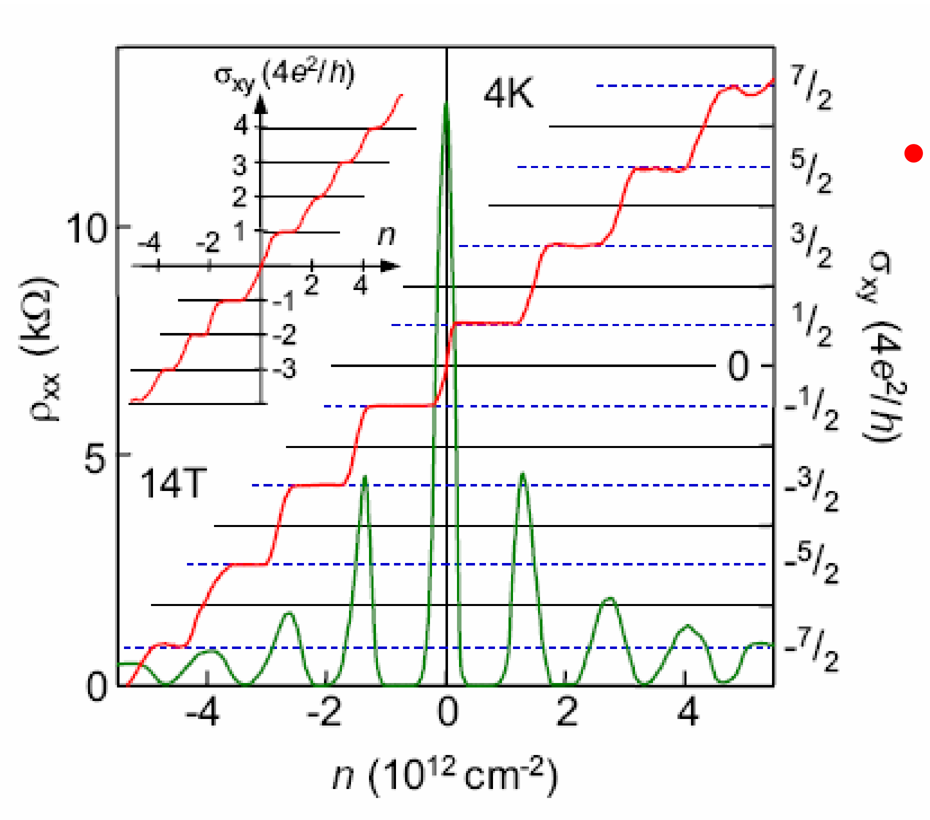
- Γ = 8×8 Dirac Matrices (diagonal in spin and K point indices)

$$\Gamma^x = \sigma^x_{aa'}\tau^z_{\alpha\alpha'}\delta_{ss'} \qquad \Gamma^y = \sigma^y_{aa'}\delta_{\alpha\alpha'}\delta_{ss'}$$

- Sublattice index plays role of "pseudospin" for Dirac equation

Electrical Measurements on Graphene

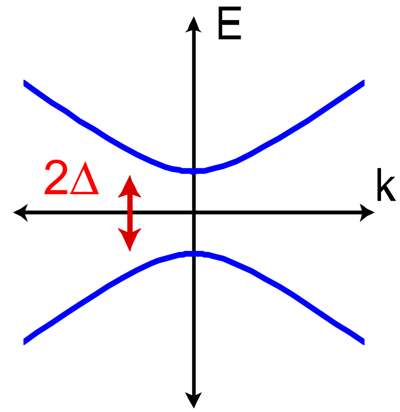
Novoselov et al. &
Zhang, et al. Nature 2005



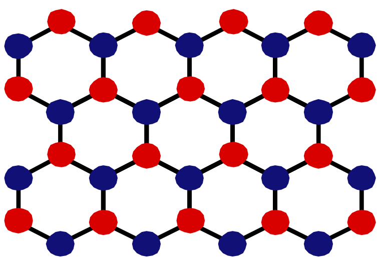
- B=0 conductivity :
  - n or p type upon gating.
  - High mobility ~ 10^4 cm^2/Vs
- B>0 : Quantum Hall Effect Observed
  - σ_{xy} quantized in half integer multiples of $4e^2/h$.
  - "Half quantized" : Consequence of Graphene's Dirac electronic structure. Berry's phase for Dirac fermions

Energy Gaps: lift degeneracy at K

$$E(p) = \pm\sqrt{v_F^2 p^2 + \Delta^2}$$



1. Staggered Sublattice Potential (e.g. BN)

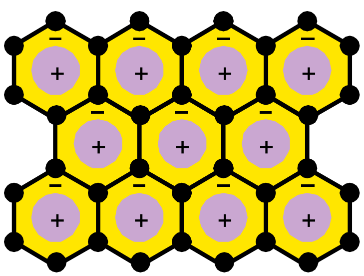


$$V = \Delta_{CDW}\sigma^z$$

Broken Inversion Symmetry

Leads to a Band Insulator

2. Periodic Magnetic Field with 0 net flux (Haldane PRL '88)



$$V = \Delta_{\text{Haldane}}\sigma^z\tau^z$$

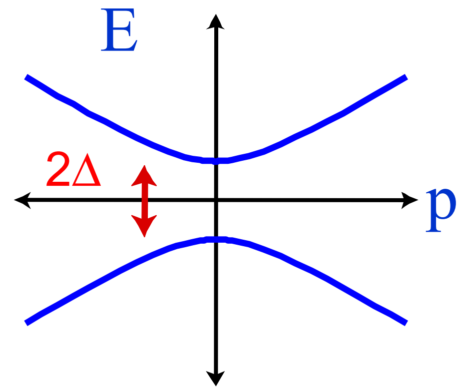
Broken Time Reversal Symmetry

Leads to Quantized Hall Effect

$$\sigma_{xy} = e^2/h$$

Both terms violate symmetries (P & T) present in graphene

3. Intrinsic Spin Orbit Potential



$$V = \Delta_{SO}\sigma^z\tau^z s^z$$

Respects ALL symmetries of Graphene, and WILL BE PRESENT. An ideal sheet of graphene has an intrinsic energy gap

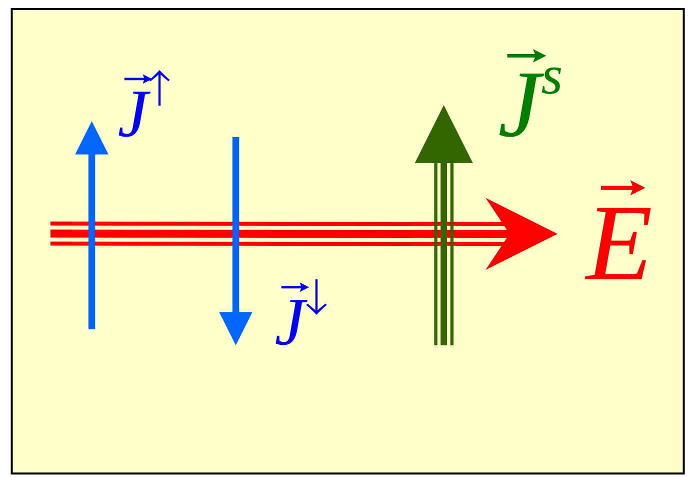
↑ and ↓ spins are independent : " (Haldane)^2 "

Leads to Quantum Spin Hall Effect for μ,T << Δ_{so}

$$\vec{J}^{\uparrow\downarrow} = \pm\frac{e^2}{h}\hat{z}\times\vec{E}$$

$$\vec{J}^{s} = \frac{\hbar}{2e}(\vec{J}^{\uparrow} - \vec{J}^{\downarrow}) = \sigma_{xy}^{s}\hat{z}\times\vec{E}$$

$$\sigma_{xy}^{s} = \frac{e}{2\pi}\mathrm{sgn}(\Delta_{SO})$$



The spin-orbit energy gap defines a time reversal invariant "topological insulator" phase of matter that is distinct from an ordinary insulator.

The Spin Orbit Gap in Graphene is small :

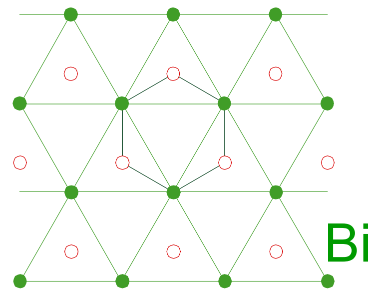
- Nearly Free Electron estimate (1st order) : $2\,\Delta_{so} \sim 15$ K
- Tight binding estimate (2nd order), pseudopotential : $2\,\Delta_{so} \sim 10$ mK

Min, et al. '06, Yao et al. '06

QSH effect predicted in materials with strong spin orbit interactions :

- Bismuth bilayer (Murakami PRL 06)

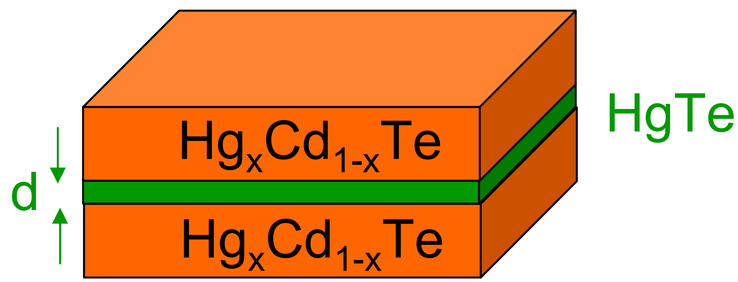
  QSH phase predicted with $2\,\Delta_{so} \sim 1000$ K



- HgTe/CdTe Heterostructure (Bernevig, Hughes, Zhang, Science 06)

  HgTe has inverted bandstructure at Γ
  2D Quantum well exhibits QSH phase

  $2\,\Delta_{so} \sim 200$ K for $d \sim 70$ Å.



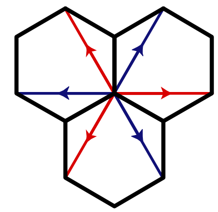
- 3D Materials (Fu, Kane '06)

  α-Sn, HgTe under uniaxial strain, and $Bi_x\,Sb_{1-x}$

"Spin Filtered" Edge States

Tight binding model:

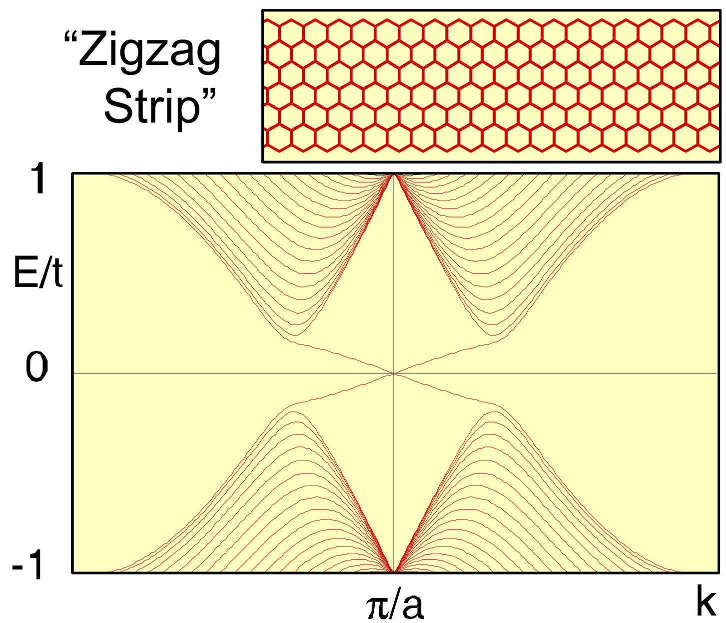
$$H = t \sum_{\langle i,j \rangle} c_i^\dagger c_j + i\lambda_{SO} \sum_{\langle\langle i,j \rangle\rangle} \nu_{ij} c_i^\dagger s^z c_j$$



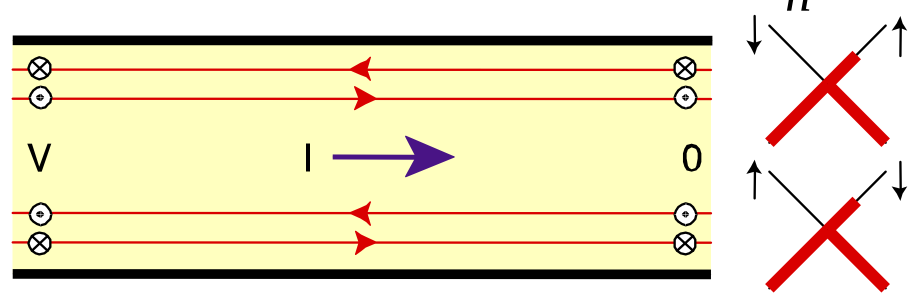
$$\vec{s} \cdot (\vec{d}_1 \times \vec{d}_2)$$

$$\Delta_{SO} = 3\sqrt{3} t_2$$

$$\nu_{ij} = -\nu_{ji} = +1(-1)$$



Two Terminal Conductance: $I = 2\frac{e^2}{h}V$



Charge Transport = Spin Accumulation

$$\rho_{\mathrm{Spin}} = n_{R\uparrow} - n_{L\downarrow} = J_{\mathrm{Charge}} / \mathrm{v_F}$$

$$\rho_{\mathrm{Charge}} = n_{R\uparrow} + n_{L\downarrow} = J_{\mathrm{Spin}} / \mathrm{v_F}$$

"Half" an ordinary 1D electron gas

Beyond The (Haldane)^2 Model

S_z is NOT actually conserved. Violations will arise from:

- Rashba Interaction (broken mirror symmetry due to substrate)

$$V = \lambda_R \hat{z} \cdot (\vec{S} \times \vec{p})$$

- Multiband effects (e.g. $p_{x,y}$ orbitals) :

$$V = \alpha \vec{L} \cdot \vec{S}$$

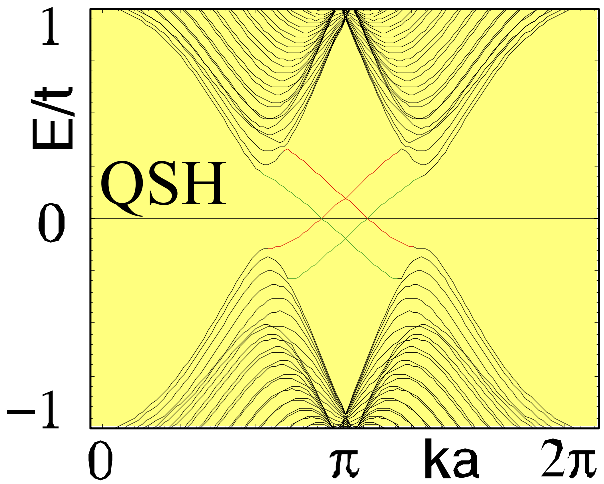
- Electron-Electron Interactions

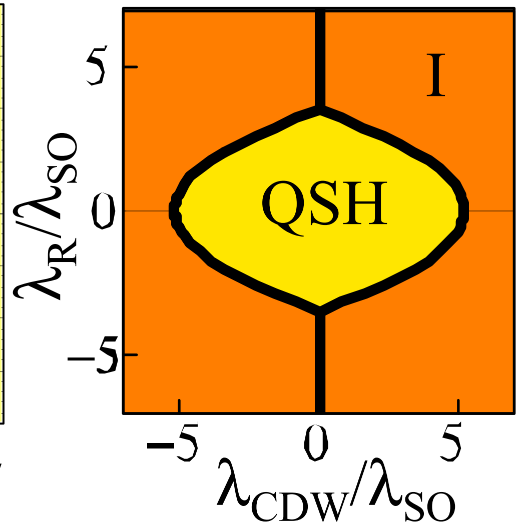
Is the QSH state distinguishable from a simple insulator ?

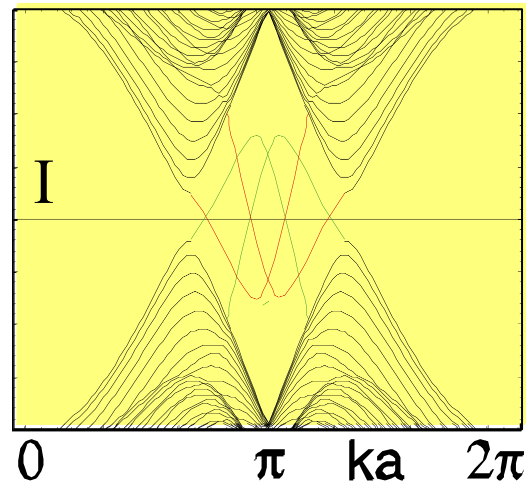
- YES
- Important role played by TIME REVERSAL symmetry
- Gapless edge states persist, but spin Hall conductivity is no longer precisely quantized (though the correction is small).

The Quantum Spin Hall Phase

- Include Rashba term λ_R and staggered sublattice potential λ_{CDW}
- QSH phase persists even when S_z is not conserved







QSH Phase

- Single pair of time reversed edge states traverse gap on each edge
- Crossing of edge states at π protected by time reversal symmetry
- Elastic Backscattering forbidden by time reversal. No localization

Insulating (I) Phase

- Edge states do not traverse gap, or in general localized
- QSH and I phases are distinguished by number of edge state pairs mod 2

Topological Invariant

- Integer Quantum Hall Effect   Thouless, et al. (TKNN) (1982)

  Hall conductivity is a Chern invariant, $\sigma_{xy}=ne^2/h$,

$$n = \frac{1}{2\pi i}\int_{BZ} d^2\mathbf{k} \cdot \langle \nabla_{\mathbf{k}} u(\mathbf{k}) | \times | \nabla_{\mathbf{k}} u(\mathbf{k}) \rangle$$

- Spin Conserving (Haldane)^2 Model

  - Independent TKNN invariants: $n_\uparrow \; , n_\downarrow$
  - Time Reversal Symmetry : $n_\uparrow + n_\downarrow = 0$
  - Spin Hall conductivity : $n_\uparrow - n_\downarrow \neq 0$

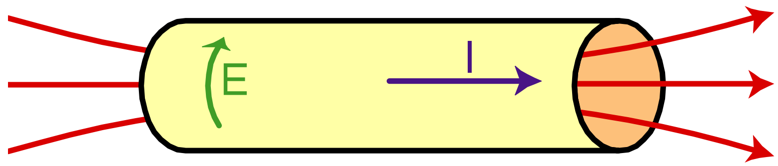
- Quantum Spin Hall Phase (without spin conservation)

  - The single defined TKNN integer is ZERO.
  - QSH phase characterized by a new Z_2 invariant protected by time reversal symmetry.

Physical Meaning of Invariants

Sensitivity to boundary conditions in a multiply connected geometry

ν=N IQHE on cylinder: Laughlin Argument

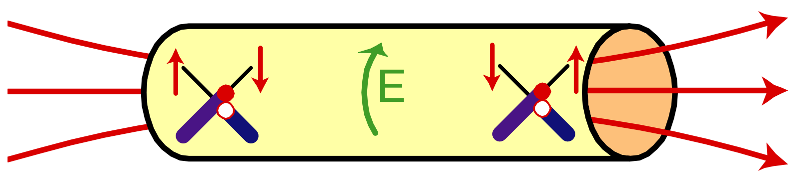


$\Delta\Phi = \phi_0$ = h/e

ΔQ = N e

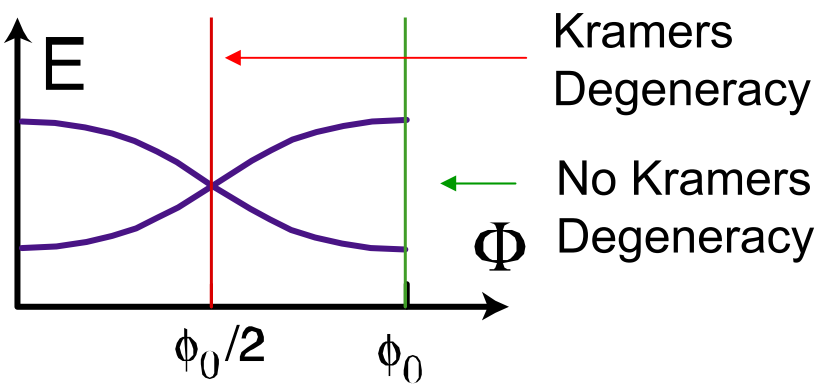
Flux $\phi_0 \Rightarrow$ Quantized change in Charge Polarization:

Quantum Spin Hall Effect on cylinder



$\Delta\Phi = \phi_0 / 2$

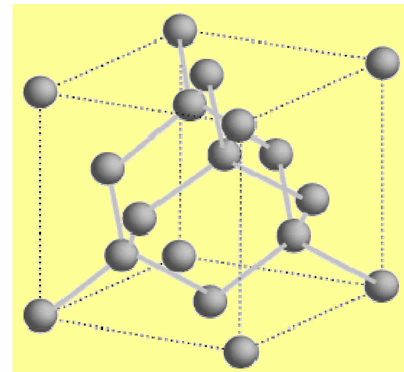
Flux ϕ_0 /2 $\Rightarrow$ Change in
“Time Reversal Polarization”,
which signals Kramers’
degeneracy at end



3D Generalization

Fu, Kane & Mele PRL, 106803 (07), cond-mat/0611341
Moore & Balents cond-mat/0607314;
Roy, cond-mat/0607531

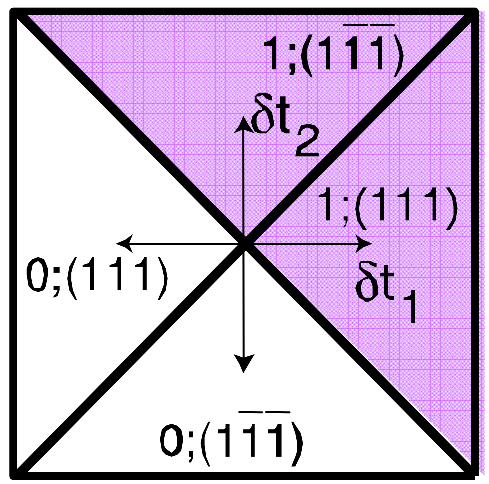
There are 4 Z_2 invariants $\nu_0;(\nu_1\nu_2\nu_3)$ distinguishing 16 "Topological Insulator" phases.



Model system: Distorted diamond lattice with spin orbit interaction

$$H = \sum_{i,a} (t + \delta t_a) c_i^\dagger c_{i+a} + i\lambda_{SO} \sum_{\ll i,j \gg} c_i^\dagger \vec{s} \cdot (\vec{d}_1 \times \vec{d}_2) c_j$$

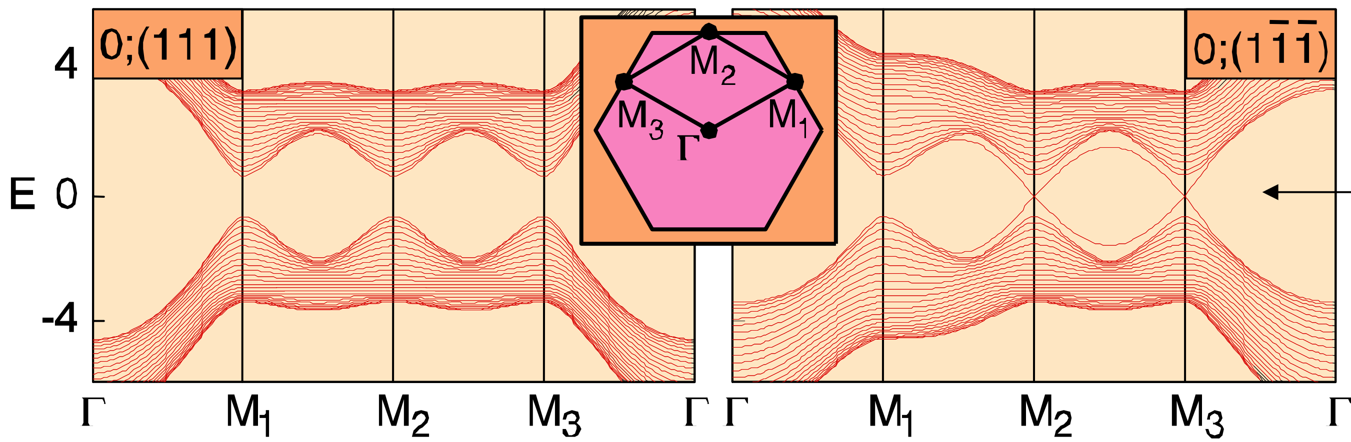
- δt_a=0 is a critical point with 3D Dirac points at 3 X points.
- δt_a (a=1,..,4) opens gaps leading to 8 different TI phases



ν_0 = 0, 1 distinguishes "weak" and "strong" topological insulators

I. Weak Topological Insulator $\nu_0 = 0$

Electronic structure of a 2D slab :

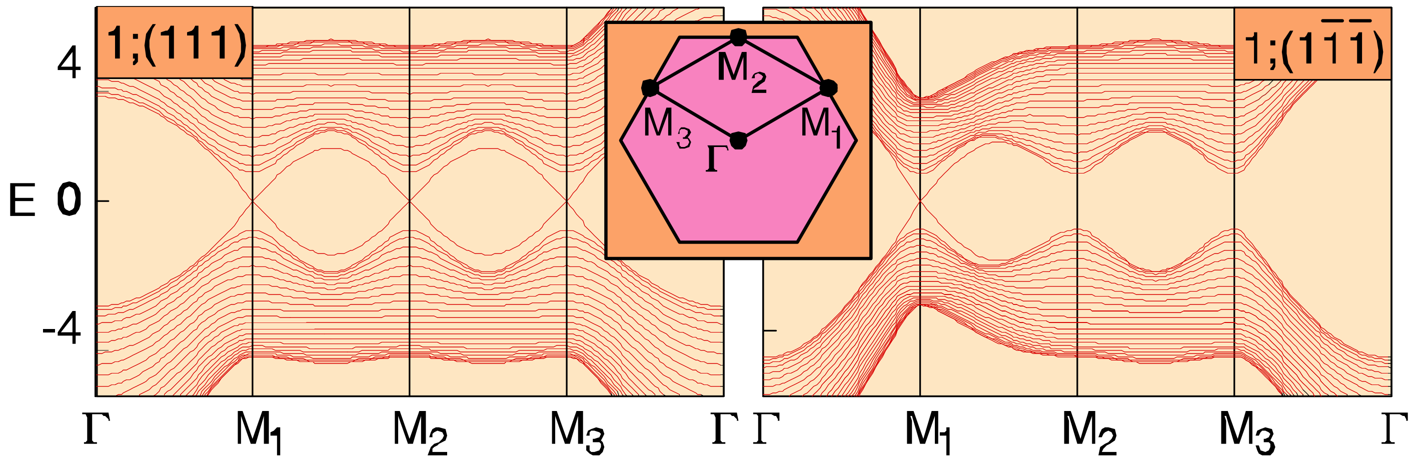


surface states with 2D Dirac points

- Equivalent to layered 2D QSH states (analogous to 3D IQHE states) stacked perpendicular to “mod 2” reciprocal lattice vector $(\nu_1\nu_2\nu_3)$.
- Each surface has either 0 or 2 2D Dirac points.
- Fragile: Disorder eliminates topological distinction.

II. Strong Topological Insulator $\nu_0 = 1$

Electronic structure of a 2D slab :



- Surface states have odd number of Dirac points on all faces.
- Robust to disorder :
  - weak antilocalization (symplectic universality class)
  - states can not be localized, even for strong disorder.
- Truly* “half quantized” QHE $\sigma_{xy} = (n+1/2)e^2/h$

Evaluating the Z_2 Invariants for Real Materials

- In general, requires knowledge of global properties of Bloch wavefunctions. Non trivial numerically.
- Enormous simplification if there is inversion symmetry:
- The Z_2 invariants can be determined from knowledge of the parity of the wavefunctions at the 8 "Time Reversal Invariant points" **k** = Γ_i that satisfy $-\Gamma_i = \Gamma_i + G$.

Parity Eigenvalue : $P|\psi_n(\Gamma_i)\rangle = \xi_n(\Gamma_i)|\psi_n(\Gamma_i)\rangle$; $\xi_n(\Gamma_i) = \pm 1$

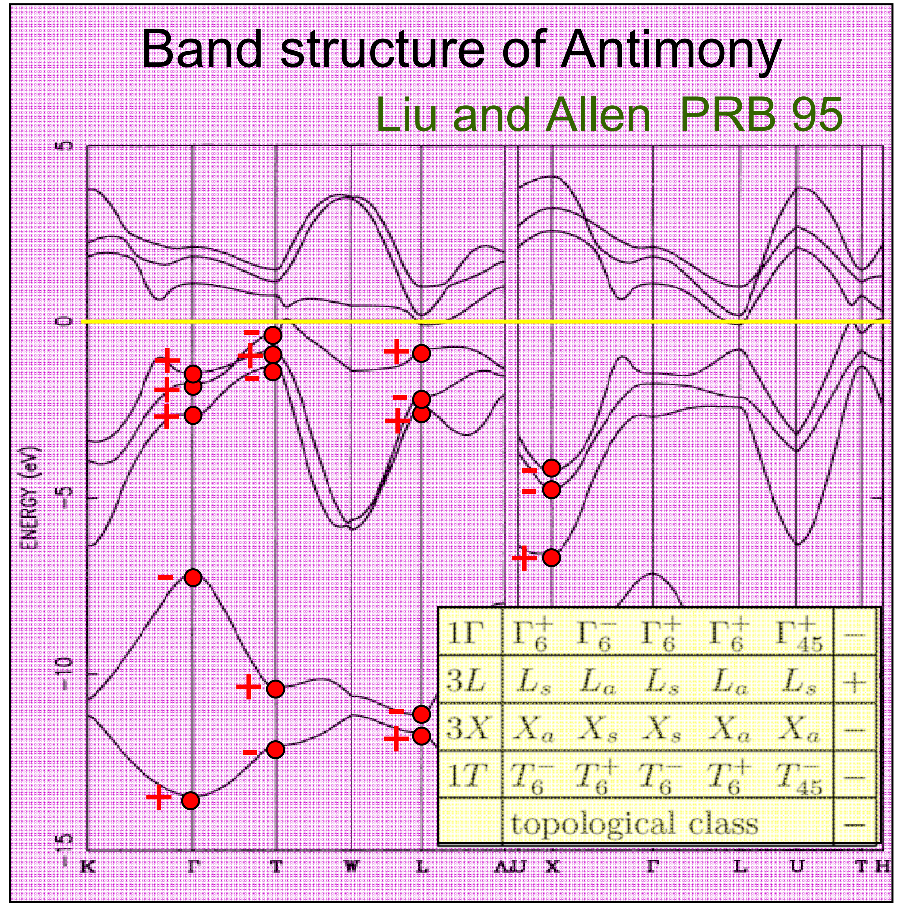
Kramers Degeneracy : $\xi_{2n}(\Gamma_i) = \xi_{2n-1}(\Gamma_i)$

"Strong" Topological Index $\nu_0 = 0 , 1$:

$$(-1)^{\nu_0} = \prod_{i=1}^{8} \prod_{n} \xi_{2n}(\Gamma_i)$$

Application : Bi_{1-x} Sb_x

- Semiconducting for .07< x < .22
- E_g ~ 30 meV at x = .18
- Occupied valence band evolves smoothly into the valence band of antimony
- Conclude $Bi_{1-x}Sb_x$ is a strong topological insulator



Other predicted strong topological insulators:

- α-Sn and HgTe under uniaxial stress
- $Pb_{1-x}Sn_xTe$ under uniaxial stress in vicinity of band inversion transition at x ~ 0.4

Conclusion

- The quantum spin Hall phase shares many similarities with the quantum Hall effect:

  - bulk excitation gap
  - gapless edge excitations
  - topological stability
  - 3D generalization

- But there are also important differences:

  - Spin Hall conductivity not quantized (but non zero).
  - Edge states are not chiral, but "spin filtered".
  - Edge transport diffusive (but not localized) at finite T.

- Open Questions :

  - Experiments on graphene? bismuth? HgCdTe? 3D materials?
  - Formulation of Z_2 invariant for interacting systems
  - Effects of disorder on surface states, and critical phenomena

Disorder and Interactions at the Edge

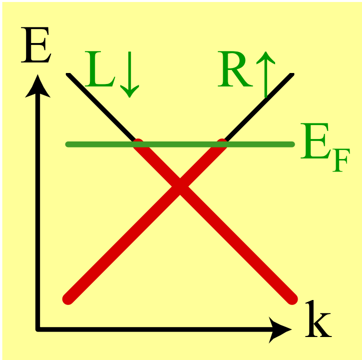
Low Energy Hamiltonian:

$$\mathcal{H} = i v_F \left(\psi^\dagger_{R\uparrow} \partial_x \psi_{R\uparrow} - \psi^\dagger_{L\downarrow} \partial_x \psi_{L\downarrow} \right) + \mathcal{H}_{\text{disorder}} + \mathcal{H}_{\text{interactions}}$$

$$\mathcal{H}_{\text{disorder}} = \left(\xi(x) \psi^\dagger_{R\uparrow} \psi_{L\downarrow} + h.c. \right) + \left(i\eta(x) \psi^\dagger_{R\uparrow} \partial_x \psi_{L\downarrow} + h.c. \right) + \ldots$$

violates time reversal

$$\mathcal{H}_{\text{interactions}} = \left(u(x)\ (\psi^\dagger_{L\downarrow} \partial_x \psi^\dagger_{L\downarrow})(\psi_{R\uparrow} \partial_x \psi_{R\uparrow}) + h.c.\ \right) + \ldots$$



Perturbative Renormalization Group Analysis : (Giamarchi & Schultz '89)

Without the leading term, $\mathcal{H}_{\text{disorder}}$ and $\mathcal{H}_{\text{interactions}}$ are irrelevant perturbations, and do not lead to a gap or to localization.

Weak interactions:

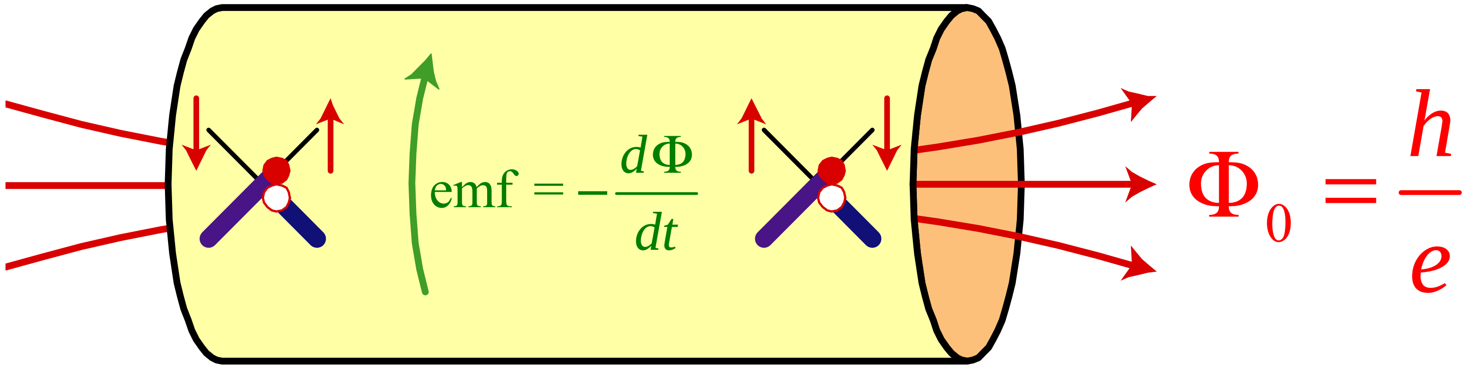
- Edge states are not localized : "absence of localization in d=1"!
- Finite 1D resistivity due to inelastic backscattering $\rho \sim T^\alpha$.

Strong interactions: (Wu, Bernevig & Zhang '05; Xu & Moore '05)

- Giamarchi - Schultz transition: Edge magnetic instability
- Spontaneously broken time reversal symmetry.

“Quantum” but not “Quantized”

Spin Hall conductance on a cylinder



- Rate of spin accumulation on edge: $\frac{d\langle S_z \rangle}{dt} = G_{xy}^s \frac{d\Phi}{dt}$
- Spin Hall Conductance $G_{xy}^s = \frac{e}{h}\left(\langle S_z \rangle_R - \langle S_z \rangle_L\right)\Big|_{E_F} \neq 0$ NOT quantized
- Spin relaxation rate ~ Inelastic backscattering rate ~ T^{α}
- For insulator no edge states, or else localized : $G_{xy}^s = 0$

Contrast with other spin Hall effects

1. Spin Hall Effect in Doped Semiconductors
   - Experiments: Kato et al. ‘05; Wunderlich et al. ‘05
   - Theory:
     Extrinsic: Dyakonov & Perel ’71; ...
     Intrinsic: Murakami, Nagaosa, Zhang ’03; Sinova et al. ’04; ...
   - Differ from QSH because there is no energy gap
2. Spin Hall Insulators Murakami, Nagaosa, Zhang ’05
   Narrow gap semiconductors, e.g. PbTe, HgTe
   - Band Insulators with large spin Hall conductivity from Kubo formula
   - Spin currents are not transport currents
   - Generically no edge states
   - No spin accumulation at edges
3. GaAs with uniform strain gradient Bernevig, Zhang ’05
   - Quantum spin Hall state with single pair of edge states.