Topological Physics in Band Insulators II

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Topological Insulators in Two and Three Dimensions

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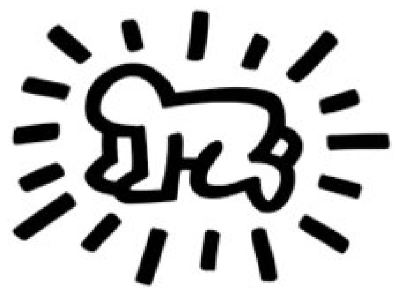
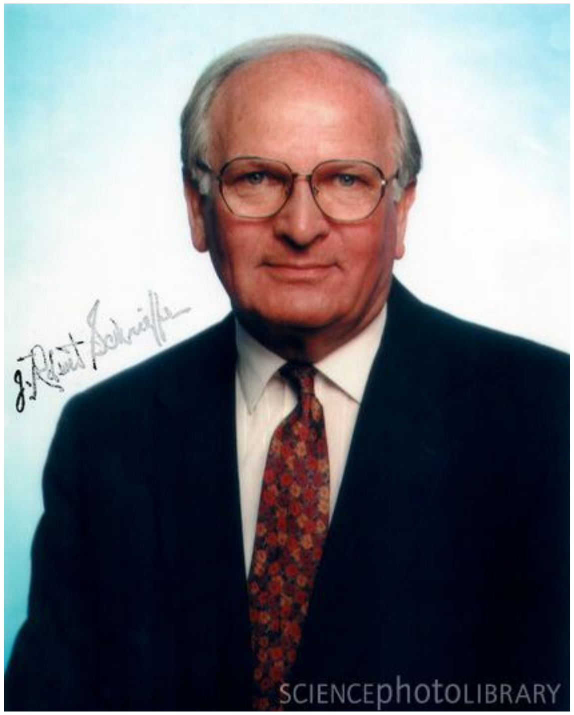
The canonical list of electric forms of matter is actually incomplete

Conductor
Insulator } 18th century

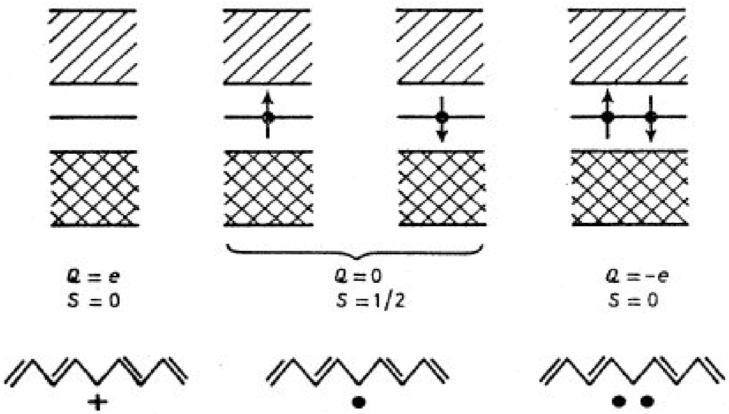
Superconductor 20th century

Topological Insulator 

Electronic States of Matter

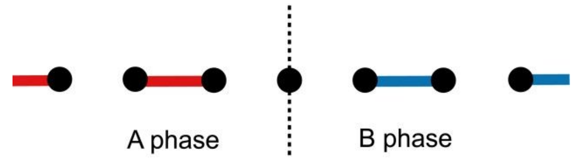


Topological Defects in $(CH)_x$

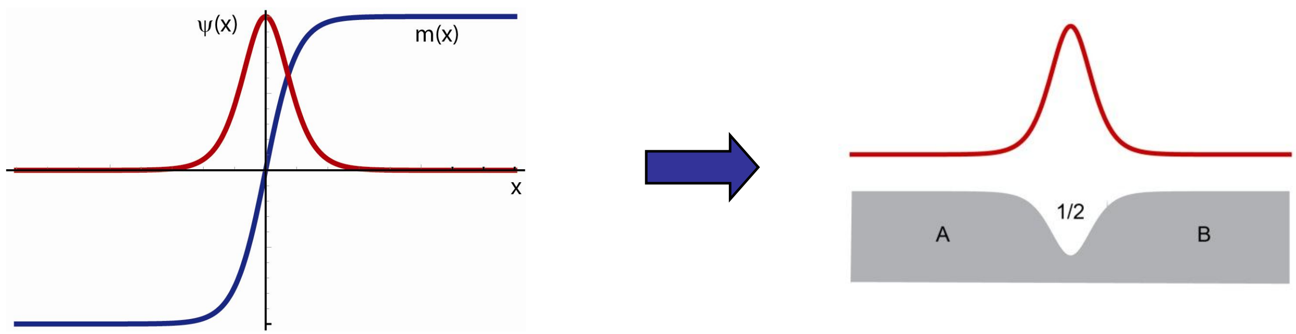


Self conjugate state from
Dirac mass inversion

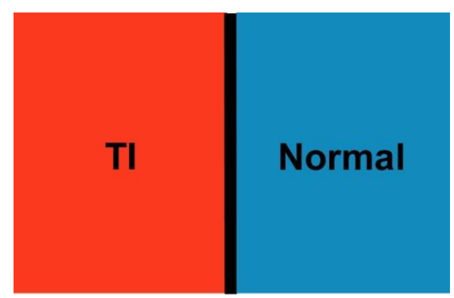
Summary of First Lecture: The unsual spin charge relation appears in the strong coupling limit, where it is a property of atoms and decoupled dimers.



This is <u>adiabatically connected</u> to a continuum limit where it arises as a transition in the ground state topology.



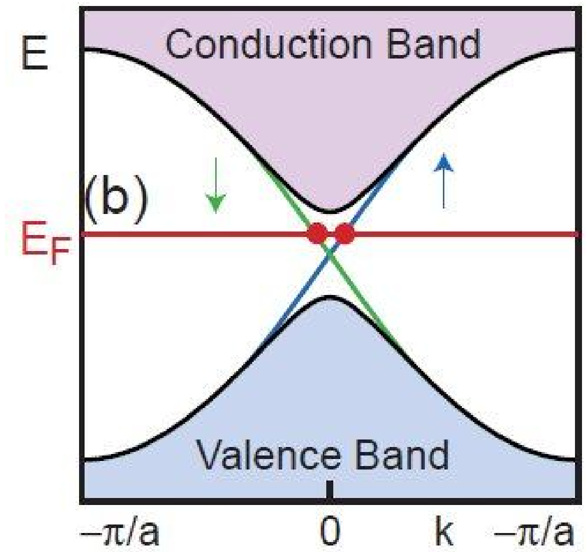
Summary of Second Lecture: This transition occurs at the boundary between a topological insulator and an ordinary insulator.



Electronic States of Matter

Topological Insulators

This novel electronic state of matter is gapped in the bulk and supports the transport of spin and charge in gapless edge states that propagate at the sample boundaries. The edge states are … insensitive to disorder because their directionality is correlated with spin.



2005 Charlie Kane and GM
University of Pennsylvania

Electron spin admits a topologically distinct insulating state

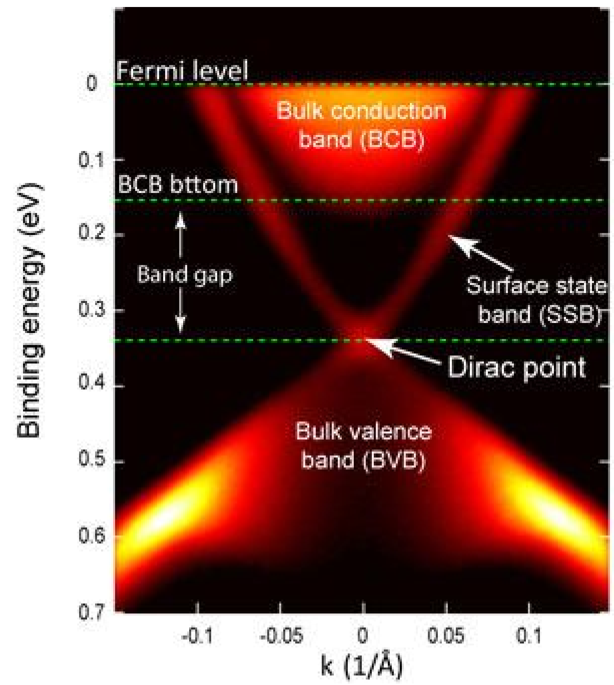
Electronic States of Matter

Topological Insulators

This state is realized in three dimensional materials where spin orbit coupling produces a bandgap “inversion.”

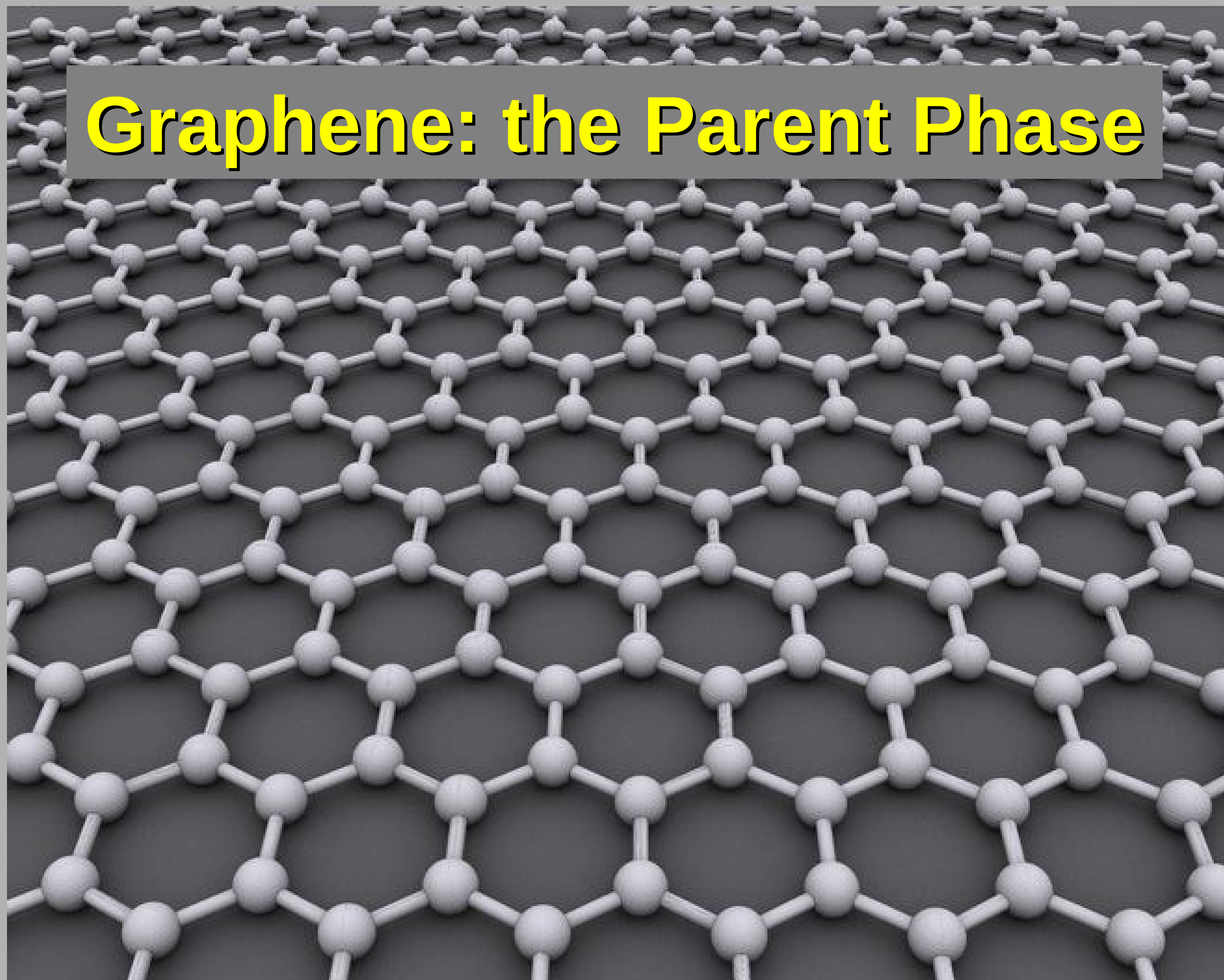
It has boundary modes (surface states) with a 2D Dirac singularity protected by time reversal symmetry.

Bi_2Se_3 is a prototype.

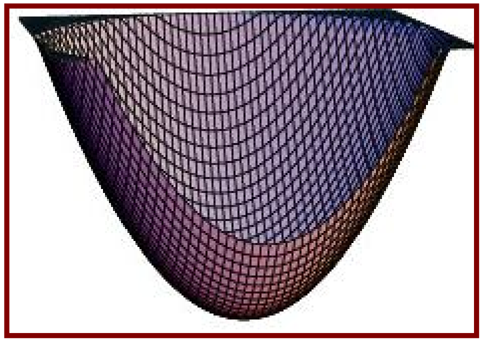


Hasan/Cava (2009)

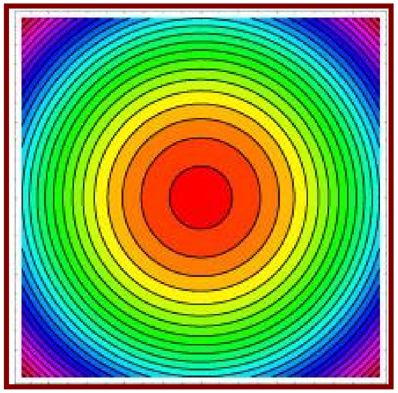
Graphene: the Parent Phase

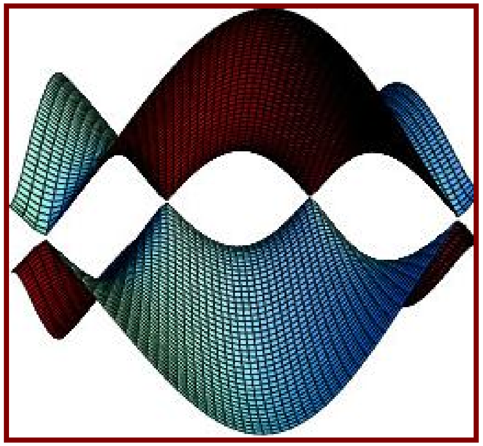


…. it has a critical electronic state

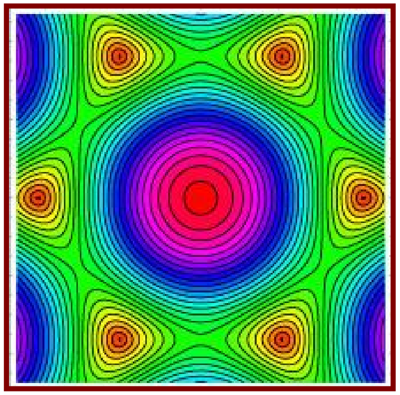


The dispersion of a
free particle in 2D..





…is replaced
by an unconventional
E(k) relation on the
graphene lattice



The low energy theory is described by an effective mass theory for massless electrons

$$\left(\textit{Bloch Wavefunction}\right) = \left(\textit{Wavefunction}(s)\ \textit{at}\ K\right) \bullet \psi(\vec{r})$$

$$H_{eff}\psi(\vec{r}) = -iv_F\left(\vec{\sigma}\bullet\nabla\right)\psi(\vec{r})$$

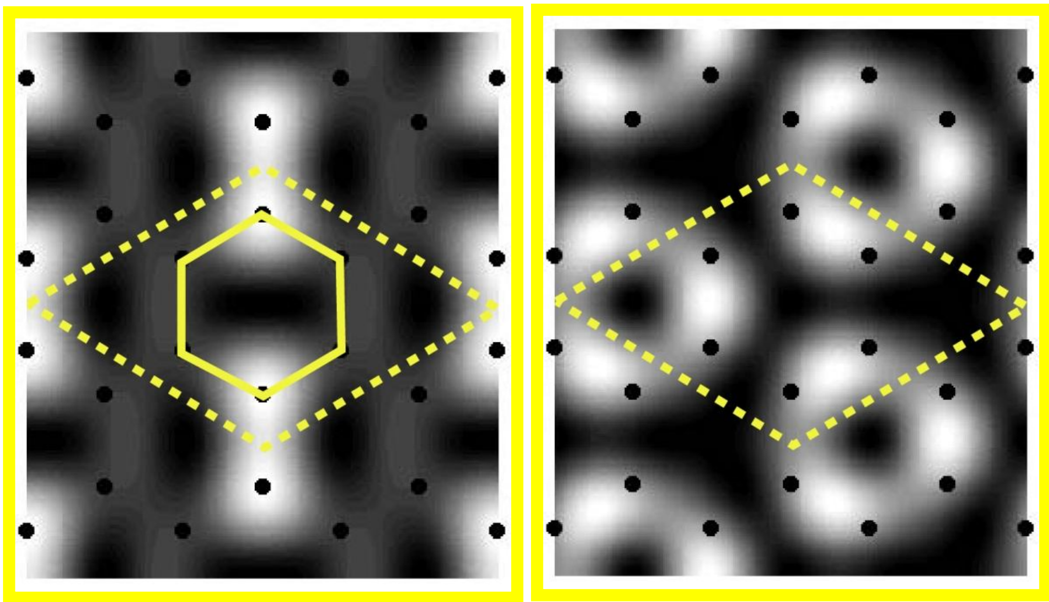
It is a massless Dirac Theory in 2+1 Dimensions

NOTE: Here the "spin" degree of freedom describes the sublattice polarization of the state, called <u>pseudospin</u>. In addition electrons carry a <u>physical</u> spin ½ and an <u>isospin</u> ½ describing the valley degeneracy.

D.P. DiVincenzo and GM (1984)

Gapping the Dirac Point

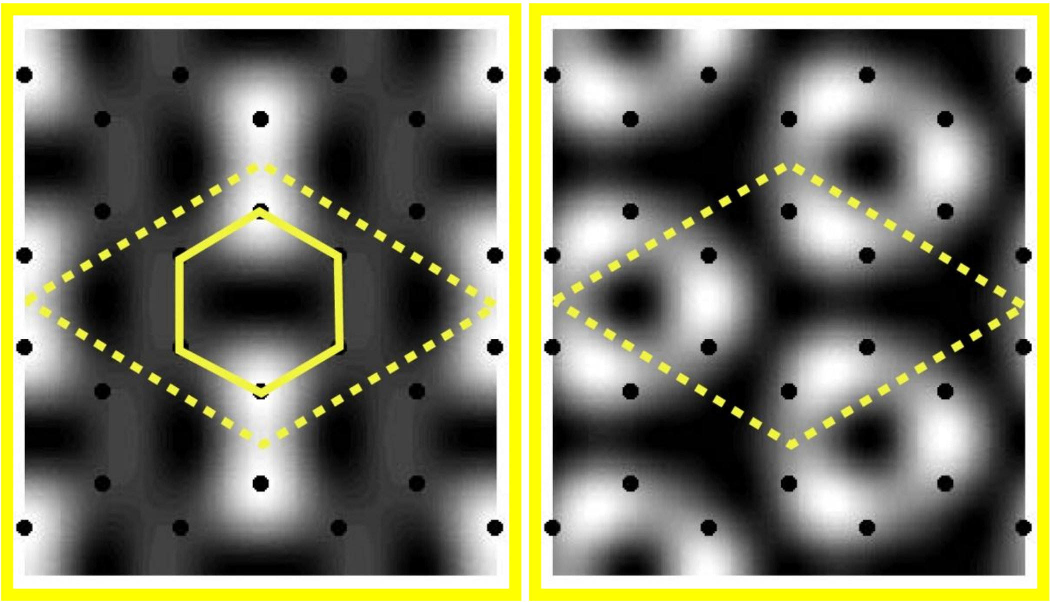
Valley mixing from broken translational symmetry



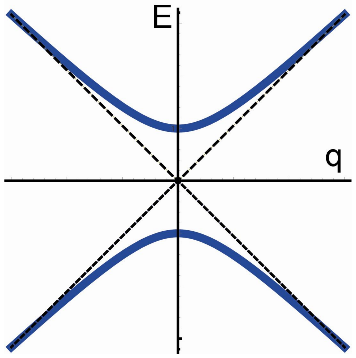
A continuum of structures all with $\sqrt{3} \times \sqrt{3}$ period hybridizes the two valleys

Gapping the Dirac Point

Valley mixing from broken translational symmetry

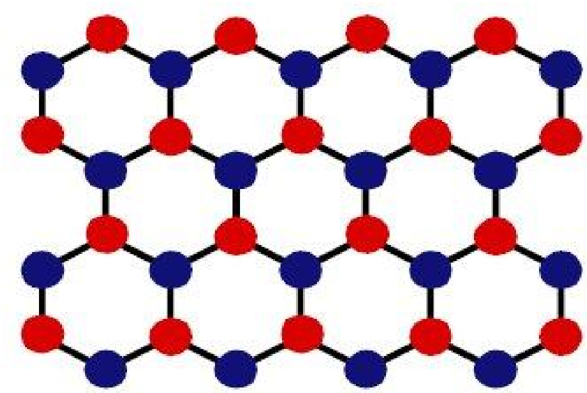


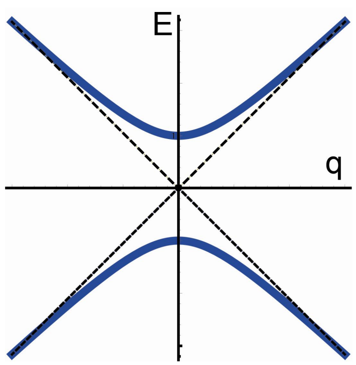
$$H' = \Delta_{\text{Kekule}} \begin{pmatrix} 0 & e^{i\vartheta}\sigma_x \\ e^{-i\vartheta}\sigma_x & 0 \end{pmatrix}_{\tau}$$



Gapping the Dirac Point

Charge transfer from broken inversion symmetry

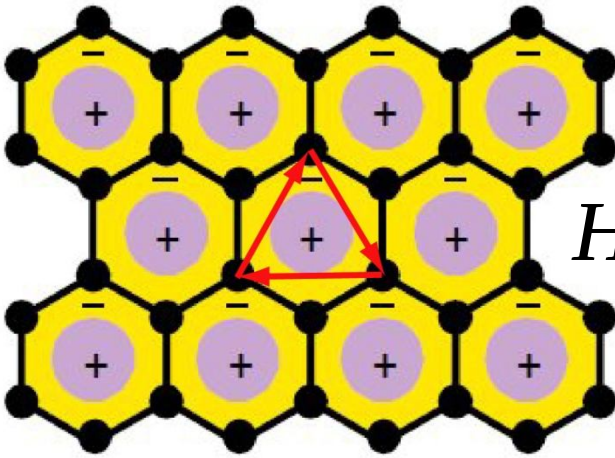




$$H' = \Delta_{\mathrm{BN}} \begin{pmatrix} \sigma_z & 0 \\ 0 & \sigma_z \end{pmatrix}_{\tau}$$

Gapping the Dirac Point

Orbital currents from modulated flux
(Broken T-symmetry)

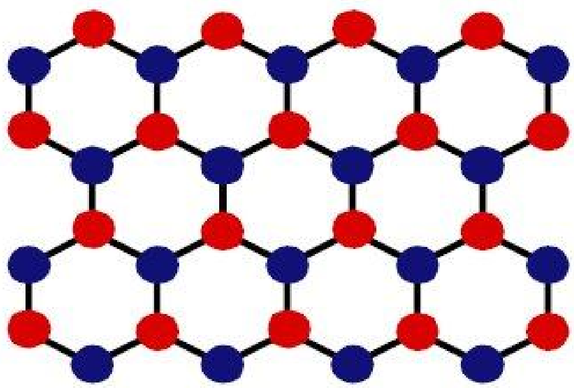


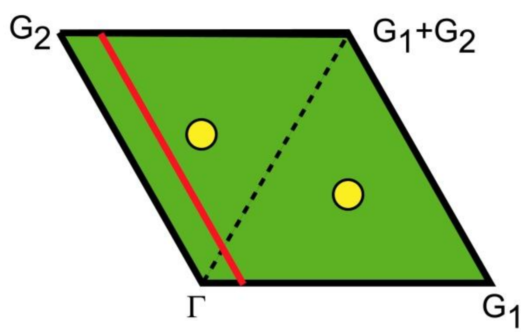
$$H' = \Delta_{\mathrm{FDMH}} \begin{pmatrix} \sigma_z & 0 \\ 0 & -\sigma_z \end{pmatrix}_\tau$$

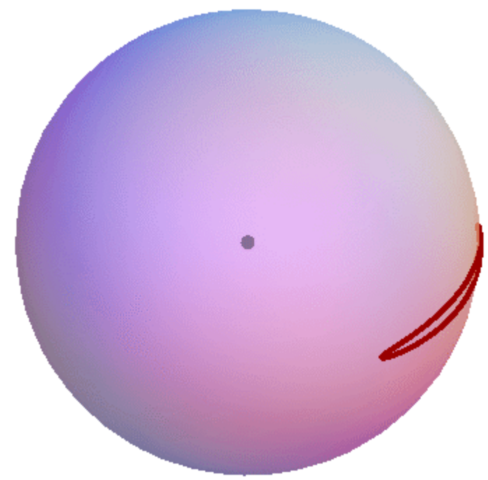
Gauged <u>second neighbor</u> hopping breaks T.
"Chern insulator" with Hall conductance e^2/h

FDM Haldane "Quantum Hall Effect without Landau Levels" (1988)

Topological Classification

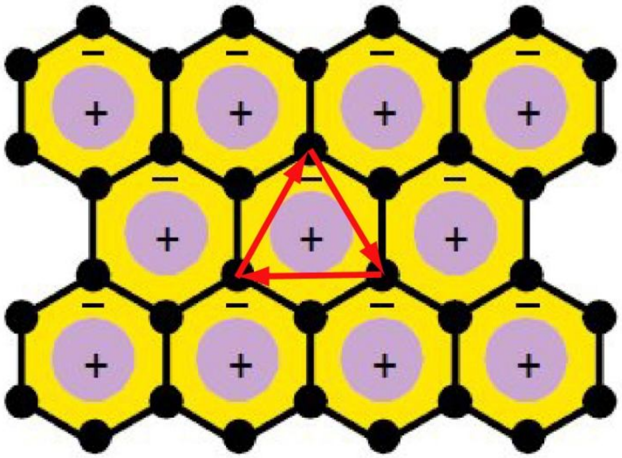


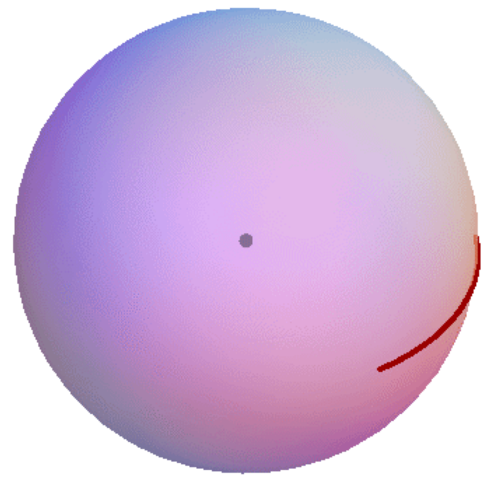




$$n = \frac{1}{4\pi}\int_S d^2k \ \left[\vec{d}(k_1,k_2)\cdot\left(\partial_{k_1}\vec{d}\times\partial_{k_2}\vec{d}\right)\right] = 0$$

Topological Classification





$$H' = \Delta_{\mathrm{FDMH}} \begin{pmatrix} \sigma_z & 0 \\ 0 & -\sigma_z \end{pmatrix}_\tau$$

$$n = \frac{1}{4\pi} \int_S d^2k \left[\vec{d}(k_1, k_2) \cdot \left(\partial_{k_1} \vec{d} \times \partial_{k_2} \vec{d} \right) \right] = 1$$

"Chern Insulator" with $\sigma_{xy} = \frac{e^2}{h}$ (has equal contributions from two valleys)

Orthodoxy: Spectrum Gapped only for Broken Symmetry States

$$H(k) = t\sum_n \cos\vec{k}\cdot\vec{a}_n\ \sigma_x + \sin\vec{k}\cdot\vec{a}_n\ \sigma_y + M\sigma_z$$

Breaks P

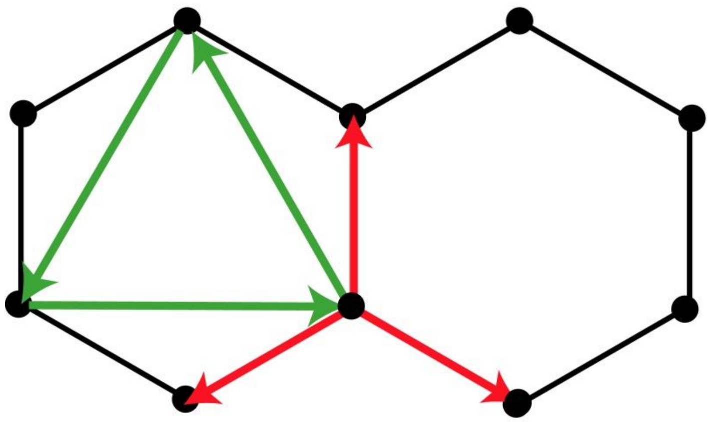
$$+2t_2 \sum_{n'} \cos\Phi\cos\vec{k}\cdot\vec{b}_{n'}\ \sigma_0 - \sin\Phi\sin\vec{k}\cdot\vec{b}_{n'}\ \sigma_z$$

Breaks e-h symmetry

Breaks T

$\{\vec{a}_n\}$: triad of nearest neighbor bond vectors

$\{\vec{b}_{n'}\}$: triad of directed "left turn" second neighbor bond vectors



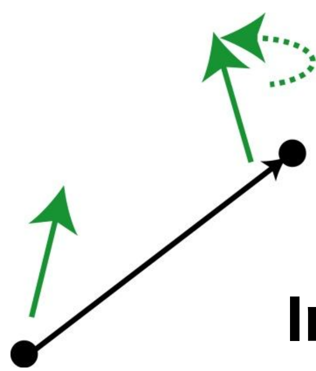
Crucially, this ignores the electron spin

Coupling orbital motion to the electron spin

Microscopic $H_{SO} = \vec{s} \cdot \nabla V \times \vec{p} \qquad V(\vec{r}) = V(\vec{r} + \vec{T})$

Lattice model $H_{SO} = i\lambda\left(\psi_m^\dagger \vec{\sigma}\psi_n - \psi_n^\dagger \vec{\sigma}\psi_m\right)\cdot \vec{\varepsilon} \times (\vec{r}_m - \vec{r}_n)$

Spin orbit field   Bond vector



Intersite hopping with spin precession

Coupling orbital motion to the electron spin

Breaking mirror symmetry with a perpendicular spin orbit field

$$\varepsilon_{xy} = 0, \varepsilon_z \neq 0 \qquad H_R = \vec{s} \cdot \varepsilon \hat{n} \times \vec{p} = -\varepsilon \hat{n} \cdot \vec{s} \times \vec{p}$$

$$-it_1 \psi_n^\dagger \left(\hat{n} \cdot \vec{s} \times \vec{d}_{mn} \right) \psi_m$$

Modifies first neighbor coupling by spin dependent potential

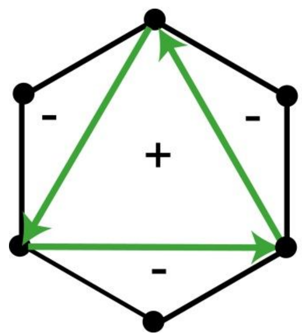
$$\Delta_R = \lambda_R \left(\sigma_x \tau_z s_y - \sigma_y s_x \right)$$

Renormalizes Fermi velocity and can fission the Dirac point

Coupling orbital motion to the electron spin

Preserve mirror symmetry with a parallel spin orbit field

$$\varepsilon_{xy} \neq 0, \varepsilon_z = 0 \qquad H_{SO} = s_z \hat{n} \cdot \vec{\varepsilon} \times \vec{p} = \vec{p} \cdot (s_z \hat{n} \times \vec{\varepsilon}) = \vec{p} \cdot \vec{a}_{eff}$$



$$\left.\begin{array}{l} \oint_{\Omega} \vec{a}_{eff} \cdot d\vec{\ell} = 0 \\ \oint_{\Omega/2} \vec{a}_{eff} \cdot d\vec{\ell} \neq 0 \end{array}\right\} \quad t_2 \left(e^{i\phi} c_n^\dagger c_m + e^{-i\phi} c_m^\dagger c_n \right) = t_2 \left[\begin{array}{l} \cos\phi \left(c_n^\dagger c_m + c_m^\dagger c_n \right) \\ \quad + i \sin\phi \left(c_n^\dagger c_m - c_m^\dagger c_n \right) \end{array} \right]$$

Generates a spin-dependent Haldane-type mass (two copies)

$$\Delta_{SO} = \lambda_{SO}\, \sigma_z \tau_z s_z$$

Mass Terms (amended)

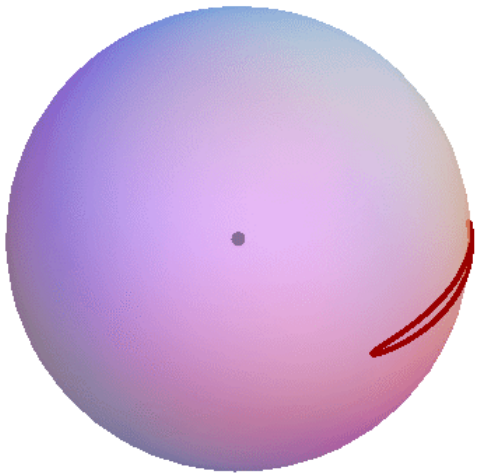
$\sigma_x\tau_x, \sigma_x\tau_y$	Kekule: valley mixing	spinless
σ_z	Heteropolar (breaks P)	spinless
$\sigma_z\tau_z$	Modulated flux (breaks T)	spinless
$\sigma_x\tau_z s_y - \sigma_y s_x$	Spin orbit (Rashba, broken z→-z)	
$\sigma_z\tau_z s_z$	Spin orbit (parallel)*	

*This term respects all symmetries and is therefore present, though possibly weak

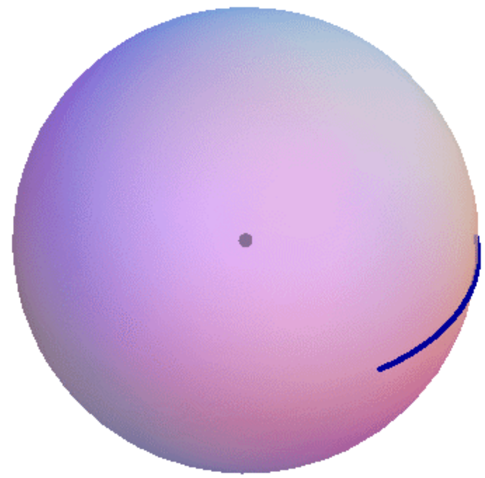
For carbon **definitely** weak, but still important

Topologically different states

Charge transfer insulator



Spin orbit coupled insulator



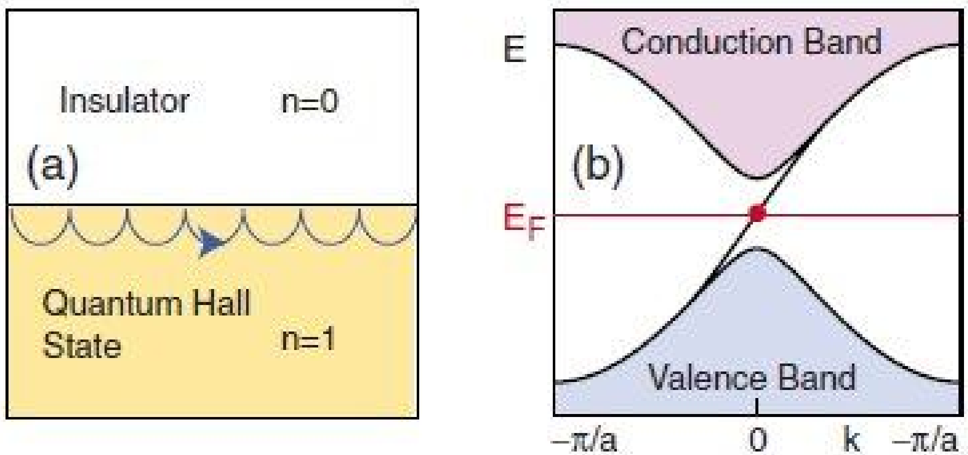
$$n = \frac{1}{4\pi} \int_S d^2k \left[\vec{d}(k_1, k_2) \cdot \left(\partial_{k_1} \vec{d} \times \partial_{k_2} \vec{d} \right) \right]$$

$$n = 0$$

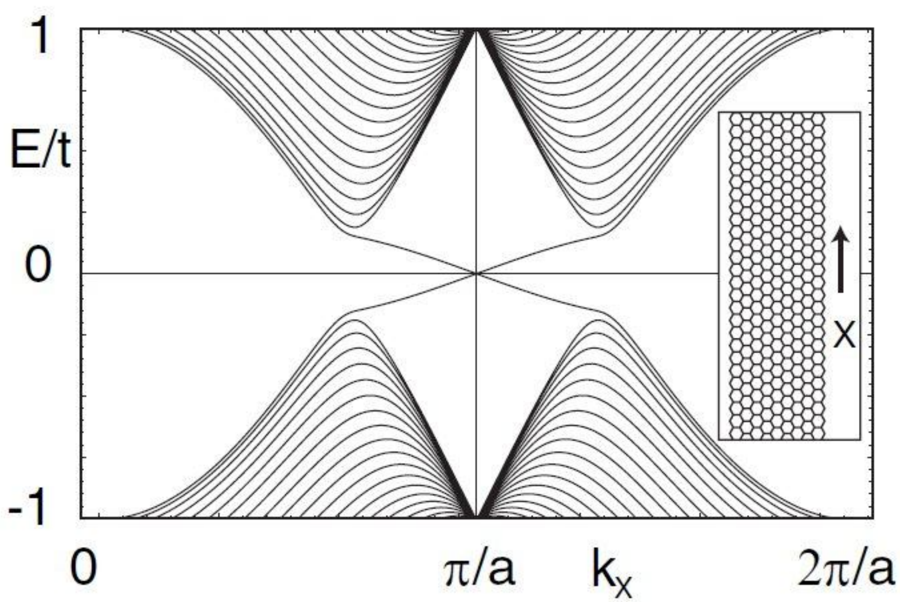
$$n = 1 + (-1) = 0$$

Topology of Chern insulator
in a T-invariant state

Boundary Modes



Ballistic propagation through one-way edge state

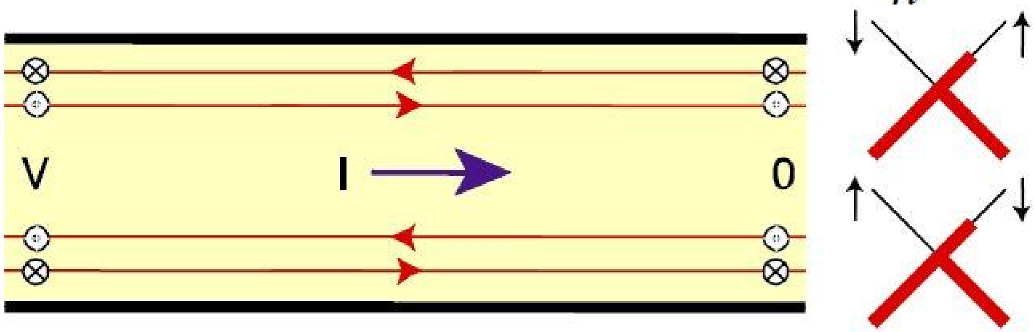


Intrinsic SO-Graphene model on a ribbon

Quantum Spin Hall Effect

Its boundary modes are spin filtered propagating surface states (edge states)

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



Charge Transport = Spin Accumulation

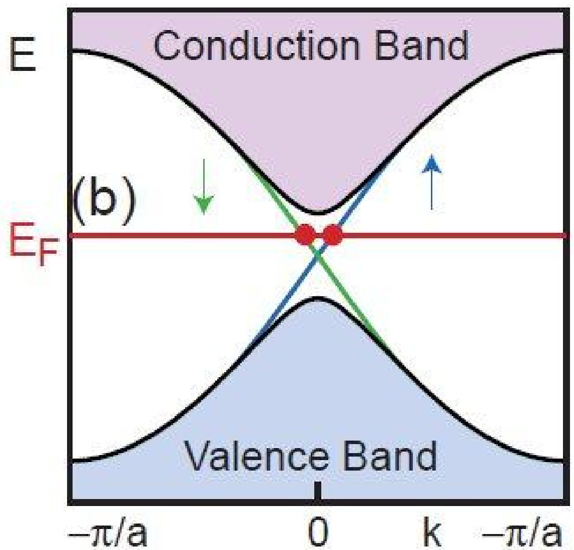
$$\rho_{\text{Spin}} = n_{R\uparrow} - n_{L\downarrow} = J_{\text{Charge}} / v_F$$

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

Comments

The H^2 model conserves S_z and is oversimplified.
Spin, unlike charge, is not conserved.

But the edge state picture is robust!



Boundary modes: Kramers pair

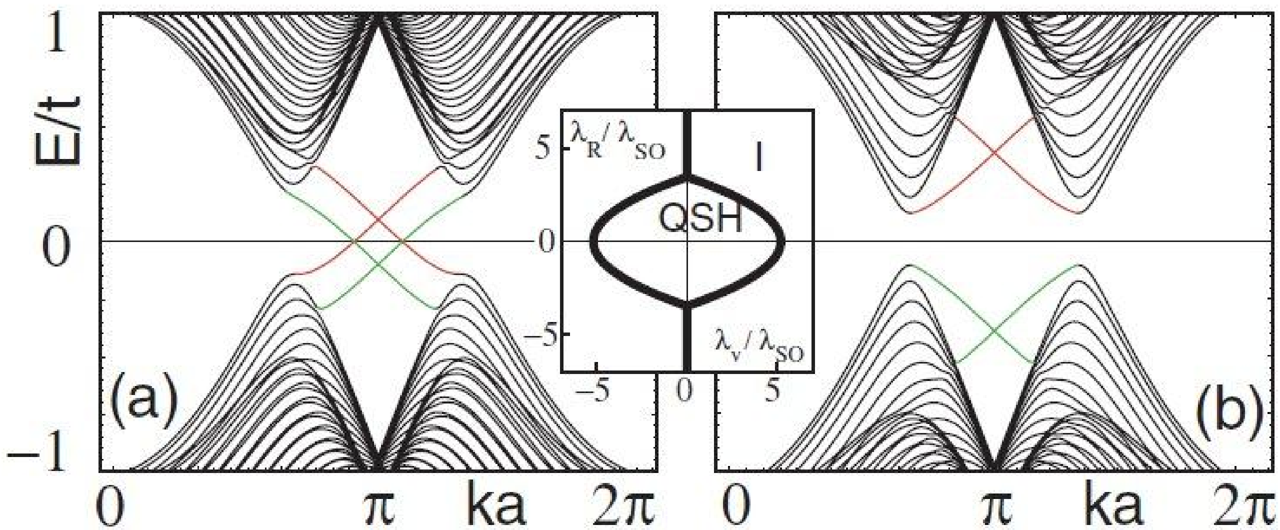
(a) Band crossing protected by T-reversal symmetry

(b) Elastic backscattering eliminated by T-symmetry

<u>Q</u>SHE: <u>q</u>uantum but not quantized

More comments

Counter-propagating surface modes reflect the bulk topological order. They can only be eliminated by a phase transition to a non-topological phase.



weak sublattice symmetry breaking

strong sublattice symmetry breaking

Symmetry Classification

Conductors: unbroken state[1]

Insulators: broken translational symmetry: bandgap from Bragg reflection[2]

Superconductor: broken gauge symmetry

Topological Insulator ?

[1]possibly with mass anisotropy

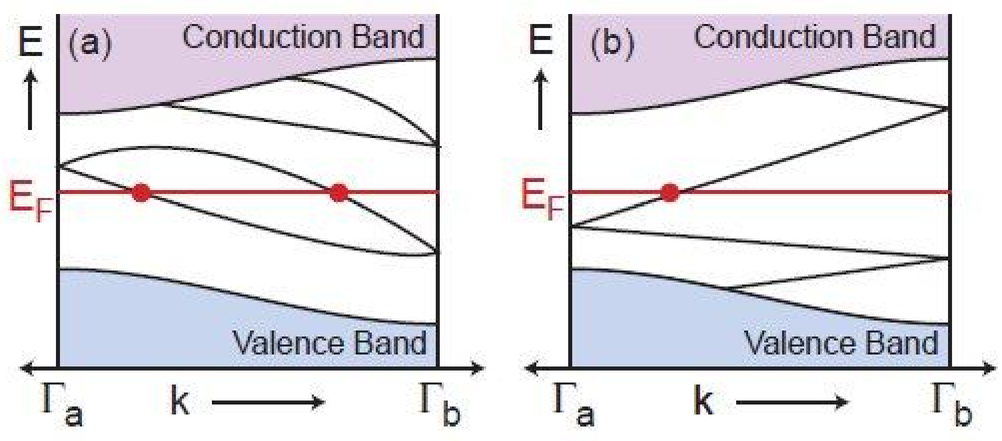
[2]band insulators

Symmetry Classification

Ordinary insulators and topological insulators are distinguished by a two-valued (even-odd) surface index.

Kramers Theorem: T-symmetry requires $E(k,\uparrow) = E(-k,\downarrow)$

But at special points k and -k are identified (TRIM)



even: ordinary (trivial)   odd: topological

Kane and GM (2005)

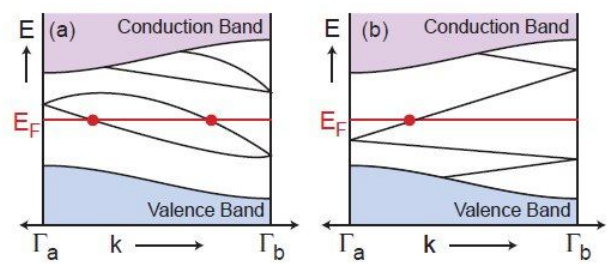
Bulk Signature

The surface modes reflect bulk topological order
distinguished by a bulk symmetry

e.g. TKKN invariant = Chern number = Hall conductance

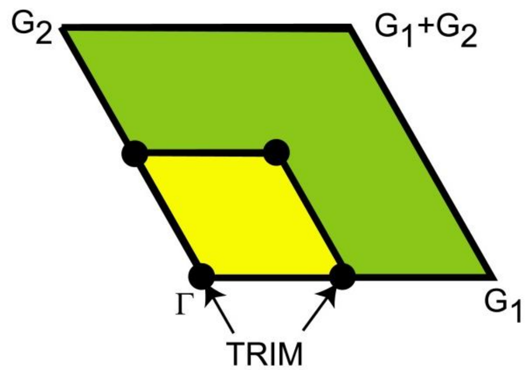
$$n = \frac{1}{4\pi} \int_S d^2k \left[\vec{d}(k_1, k_2) \cdot \left(\partial_{k_1} \vec{d} \times \partial_{k_2} \vec{d} \right) \right]$$

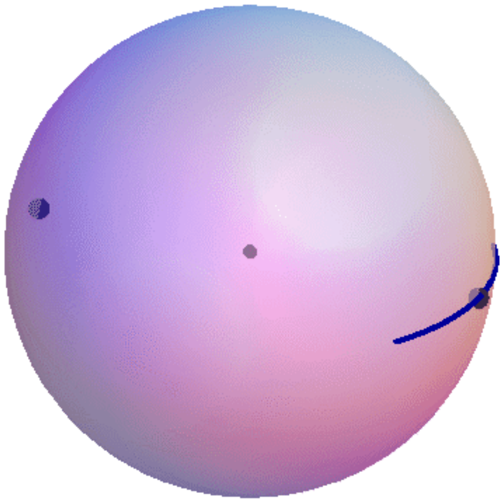
T-reversal symmetry **requires n=0**
"Spin Chern number" in S_z conserving model
is **nontopological**
TI index is **defined mod 2**



Bulk time-reversal invariant momenta

$$H\left(\frac{\vec{G}}{2}\right) = H\left(\frac{-\vec{G}}{2}\right)$$





Symmetry-protected twofold degeneracy at opposing points (**d** and –**d**) on Bloch sphere

Comparison of T reversal pairs allows topological classification of ground state

Diagnostic for Topological Order:

Periodic part of Bloch state: $u_n(\vec{k}) = e^{-i\vec{k}\cdot\vec{r}}\psi_n(\vec{k};\vec{r})$

Q. **How different are** $\left\{\Theta u_n(\vec{k})\right\}_N$ **and** $\left\{u_n(-\vec{k})\right\}_N$ **?**

A. For a trivial atomic insulator they are the **same**

A. For N bands quantify by $w_{mn}(\vec{k}) = \left\langle u_m(-\vec{k}) | \Theta | u_n(\vec{k}) \right\rangle$

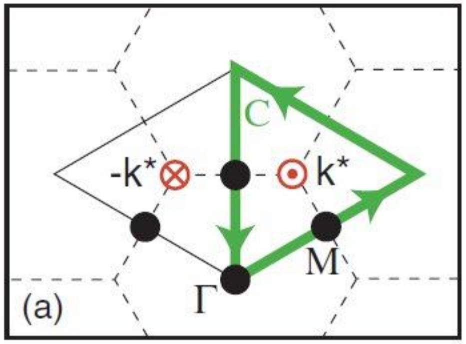
Antisymmetric: periodic complex-valued $P(\vec{k}) = \mathrm{Pf}(\mathrm{w})$

$P(\vec{k}) = 0$ {
- points (vortices) at ±k
- but never at TRIM (k=-k)

Kane and GM (2005)

Pfaffian Test

Count the zeroes of $P(\vec{k})$ in <u>one half</u> of Brillouin zone



Zero: Trivial, like an atomic insulator

Even: Adiabatically **connected** to atomic insulator by pairwise annihilation of its zeroes

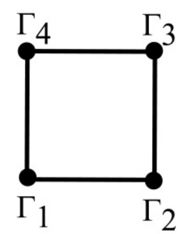
Odd: Can't be adiabatically connected to atomic insulator since $P(\vec{k})=0$ is **forbidden** at TRIM.

Direct integration requires a smooth gauge and is awkward

Pointwise Integration Rules

$$(-1)^{\nu} = \prod_a \delta_a \qquad \delta_a = \frac{\mathrm{Pf}(w(\Lambda_a))}{\sqrt{\det w(\Lambda_a)}} = \pm 1$$

Track sign changes of δ's between TRIM



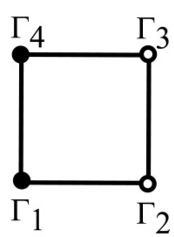
Atomic insulator: all $\delta_a > 0$ (or < 0)

$\delta_a \delta_b < 0$: exchange Kramers partners

Gauge Invariant Products: $\delta_{a_1}\delta_{a_2}\delta_{a_3}\delta_{a_4} < 0$

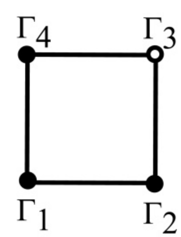
$\prod_a \delta_a > 0$:

"conventional"



$\prod_a \delta_a < 0$:

"topological"

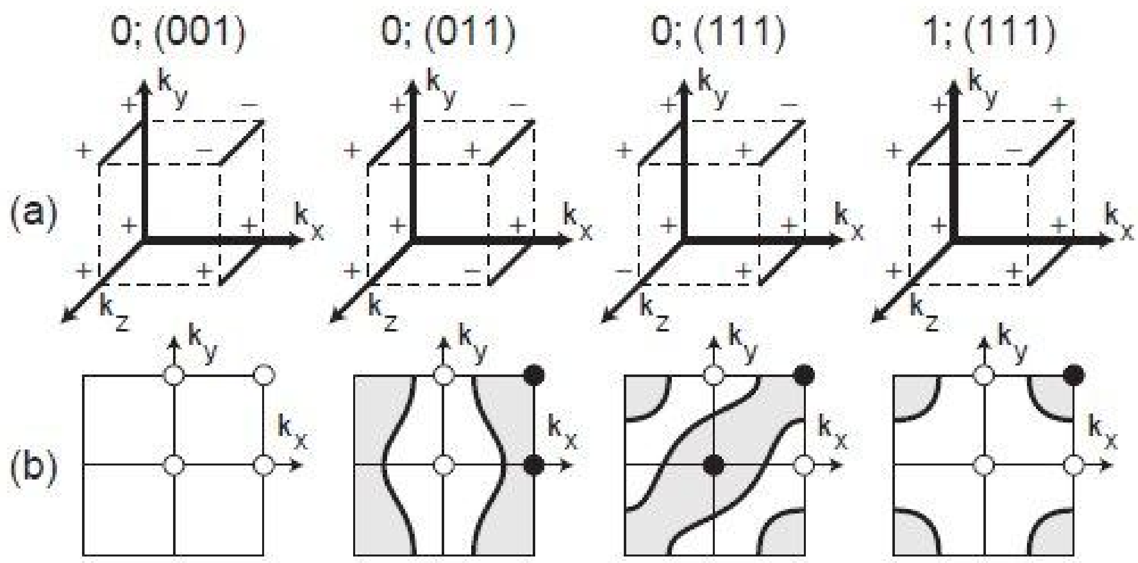


Fu, Kane and GM (2007)

With inversion symmetry

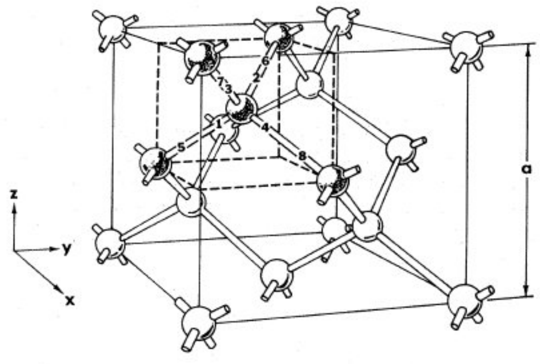
Ordinary insulators and topological insulators are distinguished by a two-valued (ν = 0,1) bulk index.

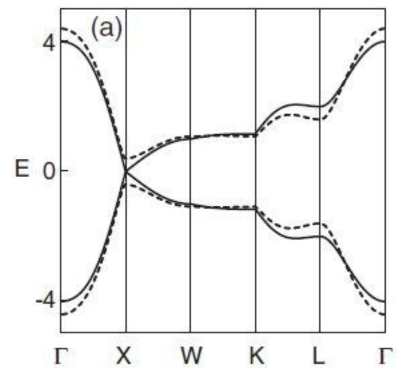
$$(-1)^{\nu} = \prod_{a=1}^{N} \delta_a \qquad \delta_a = \prod_m \xi_m$$ (parity eigenvalues, ±1)

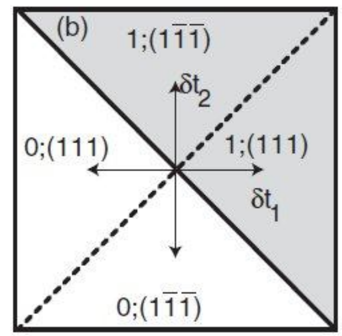


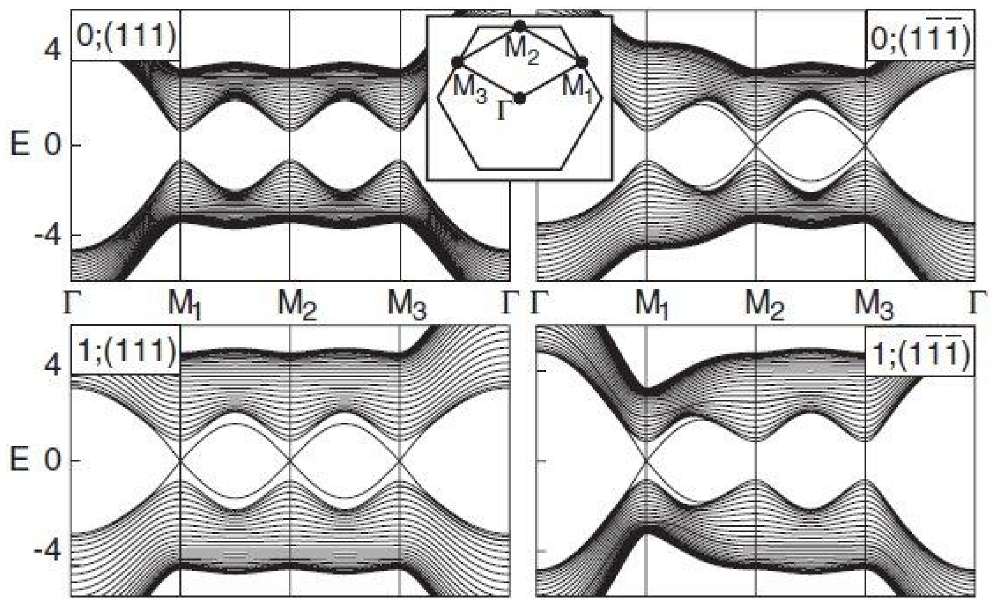
Fu, Kane and GM (2007)

Example: one orbital diamond lattice





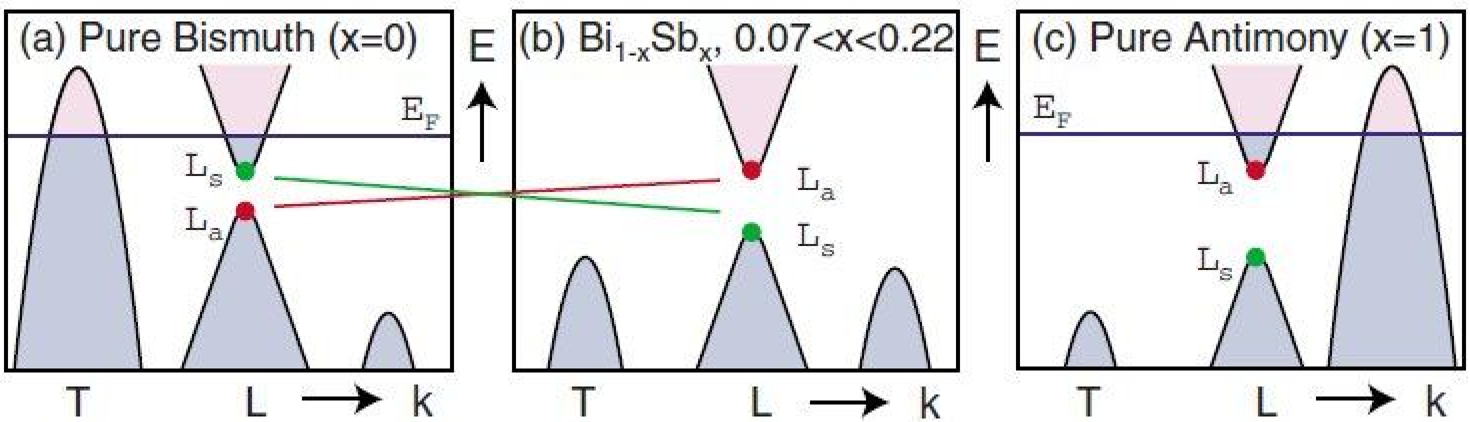




Example: Bi_xSb_{1-x}

TABLE II. Symmetry labels for the Bloch states at the 8$\mathcal{T}$ invariant momenta Λ_a for the five valence bands of Bi and Sb. δ_a's are given by Eq. (12) and determine the topological class $(\nu_0;\nu_1\nu_2\nu_3)$ by relations similar to Eq. (10). The difference between Bi and Sb is due to the inversion of the L_s and L_a bands that occurs at $x \sim 0.04$.

Bi: Class (0;000)							Sb: Class (1;111)						
Λ_a	Symmetry label					δ_a	Λ_a	Symmetry label					δ_a
1Γ	Γ_6^+	Γ_6^-	Γ_6^+	Γ_6^+	Γ_{45}^+	−1	1Γ	Γ_6^+	Γ_6^-	Γ_6^+	Γ_6^+	Γ_{45}^+	−1
$3L$	L_s	L_a	L_s	L_a	L_a	−1	$3L$	L_s	L_a	L_s	L_a	L_s	+1
$3X$	X_a	X_s	X_s	X_a	X_a	−1	$3X$	X_a	X_s	X_s	X_a	X_a	−1
$1T$	T_6^-	T_6^+	T_6^-	T_6^+	T_{45}^-	−1	$1T$	T_6^-	T_6^+	T_6^-	T_6^+	T_{45}^-	−1



Fu Kane (2007)

Some References:

Review Article: M.Z. Hasan and C.L. Kane
Rev. Mod. Phys. 82, 3045 (2010)

QSH in Graphene: C.L. Kane and E.J. Mele
Phys. Rev. Lett. 95, 226801 (2005)

Z2 insulators: C.L. Kane and E.J. Mele
Phys. Rev. Lett. 95, 146802 (2005)

Three Dimensional TI's. L. Fu, C.L. Kane and E.J. Mele
Phys. Rev. Lett. 98, 106803 (2007)

Inversion symmetric TI's. L. Fu and C.L. Kane
Phys. Rev. B 76, 045302 (2007)

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