A semi-short review on Topological insulators

Z. Hassan, C. Kane, Rev. Mod. Phys., **82**, 3045 (2010) Liang Fu and C. Kane, Phys. Rev. B, **74**, 195312 (2006) Liang Fu and C. Kane, Phys. Rev. B, **76**, 045302 (2006)

Parts of slides from Zhang's presentation in KITP School on TPI http://online.itp.ucsb.edu/online/qspinhall_m08/zhang/

Topological Insulators and Majorana modes

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Phases of matter

• Classification based on long range symmetries!





Insulators

• Maybe one of most boring phases of matter!



Intrinsic Semiconductors

2D is special for resistivity

• Scaling of resistivity $R = \rho L^{(2-d)}$

- $(e^2/h) R\;$ is dimension less in 2D

 One does not have to measure sample dimensions to have precise resistivity measurements

Quantum Hall Effect



Stormer, *Physica* **B177**, 401 (1992)



Energy gap but NOT an insulator!

$$J_{y} = \sigma_{xy} E_{x}$$
$$\sigma_{xy} = n \frac{e^{2}}{h}$$

Edge modes



Integer accurate to 10-9

Laughlin's Argument

Laughlin PRB 23, 5632



 $I = c \frac{\partial U}{\partial \phi} = \frac{c}{L} \frac{\partial U}{\partial A}$

If the states are localized just adds a phase

$$exp\left(ieAx/\hbar c\right)$$

Left: Diagram of metallic loop. Right: Density of states without (top) and with (bottom) disorder. Regions of delocalized states are shaded. The dashed line indicates the Fermi level.

When they are extended: ONLY

$$A = n \frac{\hbar c}{eL}$$

Changing A moves the center of the states from one side to the other: Change in energy

$$y_0 \to y_0 - \frac{\Delta A}{H_0}$$

$$\psi_{k,n} = e^{ikx}\phi_n(y-y_0)$$

$$\Delta U = neV \qquad I = \frac{ne^2}{h}V$$

Robust features: Topology?

The study of geometrical properties that are insensitive to smooth deformations Example: 2D surfaces in 3D

A closed surface is characterized by its genus, g = # holes



A good math book : Nakahara, 'Geometry, Topology and Physics'



Topological View of Hall Effect

Thouless et. Al., PRL 45, 405, 1982

• Periodic lattice potential:

U(x,y) Periodic in x and y with period a and b

- Magnetic Flux per unit cell: $\phi = p/q$
- Chose the gauge: $\mathbf{A} = (0, B x)$

$$H = \frac{1}{2m}(\mathbf{p} + e\mathbf{A})^2 + U(x, y)$$

$$\begin{split} \psi_{\mathbf{k}}(x+qa,y)e^{-2\pi ipy/b-ik_{x}qa} &= \psi_{\mathbf{k}}(x,y+b)e^{-ik_{y}b} = \psi_{\mathbf{k}}(x,y)\\ u_{\mathbf{k}}(x+qa,y)e^{-2\pi ipy/b} &= u_{\mathbf{k}}(x,y+b) = u_{\mathbf{k}}(x,y)\\ \text{GUAGE DEPENEDENT! Not Physical} \end{split}$$

$$u_{\mathbf{k}}(x,y) = |u_{\mathbf{k}}(x,y)| \exp[i\theta_{\mathbf{k}}(x,y)]$$
$$p = \frac{-1}{2\pi} \int d\mathbf{l} \frac{\partial \theta_{\mathbf{k}}(x,y)}{\partial \mathbf{l}}$$

Topological View of Hall Effect

$$H_{\mathbf{k}} = \frac{1}{2m} \left(-i\hbar \frac{\partial}{\partial x} + \hbar k_x \right)^2 + \frac{1}{2m} \left(-i\hbar \frac{\partial}{\partial y} + \hbar k_x - eBx \right)^2 + U(x, y)$$
$$\sigma_{x,y} = \frac{ie^2}{A\hbar} \sum_{\epsilon_{\alpha} < E_f} \sum_{\epsilon_{\beta} > E_f} \frac{(\partial H/\partial k_x)_{\alpha\beta} (\partial H/\partial k_y)_{\beta\alpha} - (\partial H/\partial k_y)_{\alpha\beta} (\partial H/\partial k_x)_{\beta\alpha}}{(\epsilon_{\alpha} - \epsilon_{\beta})^2}$$

$$\hat{\mathbf{A}}(\mathbf{k}) = \int d\mathbf{r} u_{\mathbf{k}}^{*}(\mathbf{r}) \nabla_{k} u_{\mathbf{k}}(\mathbf{r})$$
$$\sigma_{xy} = \frac{e^{2}}{2\pi h i} \int d_{k} \left[\nabla_{k} \times \hat{\mathbf{A}}(\mathbf{k}) \right]$$

Magnetic Brillouin zone is TORUS. Result not sensitive to the gauge! Non-zero results are given by non-trivial form of the phase of u_k

$$\sigma_{xy} = \frac{e^2}{h}n$$

As usual: Any simple model?

• One dimensional solid with orbital for spinless fermions



• Wave functions:

$$\ket{\eta_i} \ \ket{
u_i}$$

• Hamiltonian:

$$H = \sum_{i} \begin{bmatrix} 0 & a|\eta_i\rangle\langle\nu_i| + b|\eta_{i-1}\rangle\langle\nu_i| \\ a|\nu_i\rangle\langle\eta_i| + b|\nu_{i+1}\rangle\langle\eta_i| & 0 \end{bmatrix}$$

Periodic lattice: Momentum space!



$$\begin{bmatrix} |\eta_k\rangle \\ |\nu_k\rangle \end{bmatrix} = \sum_i e^{-ik} \begin{bmatrix} |\eta_i\rangle \\ |\nu_i\rangle \end{bmatrix} \qquad H = \sum_k \begin{bmatrix} 0 & (a+e^{-ik} b) |\eta_k\rangle \langle \nu_k| \\ (a+e^{ik} b) |\nu_k\rangle \langle \eta_k| & 0 \end{bmatrix}$$

$$H_k = [a + b \ Cos(k)] \sigma_x + b \ Sin(k)\sigma_y$$

$$E(k) = \pm \sqrt{a^2 + b^2 + 2ab \ Cos(k)}$$



Band inversion

$$H_k = [a + b \, Cos(k)] \, \sigma_x + b \, Sin(k) \sigma_y$$

Time Reversal

$$\Theta k = -k$$

$$H_0 = [a+b] \sigma_x, \ H_\pi = [a-b] \sigma_x$$

Inversion



$$P \ k = -k \qquad P \equiv \sigma_x$$

$$p = \pm 1$$
 $E_0 = \pm (a+b), E_\pi = \pm (a-b)$

At k = 0 lower band p = -1At $k = \pi$ lower band parity depends on (a-b)



What is happening?

Edge modes appear when parity changes!





Chiral edge states

• Experimental signature on the edge Chern-Simon field theory with signatures on the edge!



No Back scattering: ANTI-LOCALIZATION

Extreme magnetic field! Broken time reversal! Anything simpler? AND in dimensions higher than ONE!

Zhang, KITP 2008

With time reversal??

Chiral (QHE) and helical (QSHE) liquids in D=1





The QHE state spatially separates the two chiral states of a spinless 1D liquid

The QSHE state spatially separates the four chiral states of a spinful 1D liquid



No go theorems: chiral and helical states can never be constructed microscopically from a purely 1D model Wu, Bernevig, Zhang; Nielsen, Ninomiya

Time reversal is SPECIAL!

Time-reversal T is defined as:

$$\langle T\psi | T\phi \rangle = \langle \phi | \psi \rangle$$

for any two states $\phi \& \psi$. It says that the inner product of the time-reversed states is the complex conjugate of the inner product of the original states. For fermions, $T^2 = -1$. If $|\phi\rangle = |T\psi\rangle$, then,

$$\begin{aligned} \langle \psi | \phi \rangle &= - \langle T^2 \psi | \phi \rangle \\ &= - \langle T(T\psi) | T\psi \rangle \\ &= - \langle T\phi | T\psi \rangle \\ &= - \langle \psi | \phi \rangle \end{aligned}$$

so $\langle \psi | \phi \rangle = 0$. Similarly, if some hermitian operator V preserves time-reversal, then $TVT^{-1} = V$ or [T, V] = 0. So,

$$\begin{aligned} \langle \psi | V | \phi \rangle &= \langle \psi | V | T \psi \rangle \\ &= \langle \psi | T V \psi \rangle \\ &= - \langle T^2 \psi | T V \psi \rangle \\ &= - \langle V \psi | T \psi \rangle \\ &= - \langle \psi | V | T \psi \rangle \end{aligned}$$

What is topological?



Distinct Topological features!

Spin-orbit Showing it's face!

Kramers degeneracy Protects K=0 and K= π from spliting

Ε



Band Structure of HgTe



Effective tight-binding model

Square lattice with 4-orbitals per site:

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

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

$$H_{eff}(k_x, k_y) = \begin{pmatrix} h(k) & 0 \\ 0 & h^*(-k) \end{pmatrix}$$

$$h(k) = \begin{pmatrix} m(k) & A(\sin k_x - i \sin k_y) \\ A(\sin k_x + i \sin k_y) & -m(k) \end{pmatrix} \equiv d_a(k)\tau^a$$

$$\Rightarrow \begin{pmatrix} m & A(k_x - ik_y) \\ A(k_x + ik_y) & -m \end{pmatrix}$$

Relativistic Dirac equation in 2+1 dimensions, with a mass term tunable by the sample thickness d! m<0 for $d>d_c$.

Zhang, KITP 2008



Mass domain wall

Cutting the Hall bar along the y-direction we see a domain-wall structure in the band structure mass term. This leads to states localized on the domain wall which still disperse along the x-direction.



Jackiw-Rebi

Zhang, KITP 2008

Experimental evidence



Konig et. Al. Science, 2007

Topological insulators

- Strong spin-orbit coupling: Heavy elements Small band-gap
- Preserved time reversal symmetry.
- Gapped in the bulk, gapless chiral edge modes.





3D Topological insulators

- Kramers degeneracy at TRI points
- Two ways to connect. Defined by the time-reversal polarization. Uniquely defined by the parity at TRI points



Liang Fu and C. Kane, Phys. Rev. B, 74, 195312 (2006)

Experiments

ARPES



Roushan et. al. 2009



Hsieh et. al., Xia et al. 2009

Electromagnetic response of an insulator

 Electromagnetic response of an insulator is described by an effective action:

$$S_{eff} = \frac{1}{8\pi} \int d^3x dt (\varepsilon \vec{E}^2 - \frac{1}{\mu} \vec{B}^2)$$

• However, another quadratic term is also allowed:

$$S_{\theta} = \frac{\theta}{2\pi} \frac{\alpha}{2\pi} \int d^3x dt \vec{E} \cdot \vec{B}$$

• Physically, this term describes the magneto-electric effect. Under time reversal:

$$\vec{E} \Rightarrow \vec{E} ; \vec{B} \Rightarrow -\vec{B}$$

 $\theta \Rightarrow -\theta$





4πΡ=(ε-1)**E**







4πΡ=α θ/2π **B**

4πΜ=α θ/2π Ε

θ periodicity and time reversal

- Consider an analog system of a period ring. The flux enters the partition function as:
- Therefore, the physics is completely invariant under the shift of $\Phi \Rightarrow \Phi + 2\pi n$



• Under time reversal, $\phi = >-\phi$, therefore, time reversal is recovered for two special values of ϕ , $\phi = 0$ and $\phi = \pi$.

• The ME term is a total derivative, independent of the bulk values of the fields:

$$S_{\theta} = \frac{\theta}{2\pi} \frac{\alpha}{16\pi} \int d^3x dt \epsilon_{\mu\nu\rho\tau} F^{\mu\nu} F^{\rho\tau} = \frac{\theta}{2\pi} \frac{\alpha}{4\pi} \int d^3x dt \partial^{\mu} (\epsilon_{\mu\nu\rho\sigma} A^{\nu} \partial^{\rho} A^{\tau})$$

Integrated over a spatially and temporally periodic system,

$$\int cdt \, d^3x \, \vec{E} \bullet \vec{B} = \int dx \, dy B_z \int cdt \, dz \partial_t A_z = n \Phi_0^2$$

• Its contribution to the partition function is given by $e^{i\theta n}$. Therefore, the partition function is invariant under the shift:

 $\theta \Rightarrow \theta + 2\pi n$ Time reversal symmetry is recovered at

$$\theta = 0, \quad \theta = \pi$$

$\boldsymbol{\theta}$ terms in condensed matter and particle physics

• Quantum spin chains:

$$S[\theta] = \theta \int dt dx \mathbf{n} \cdot (\partial_x \mathbf{n} \times \partial_t \mathbf{n}), \quad \theta = \frac{S}{2}$$

• Quantum Hall transitions:

 $S[\theta] = \theta \int d^2 x \epsilon^{\mu\nu} \mathrm{tr} \left(\mathbf{Q} \mathcal{D}_{\mu} \mathbf{Q} \mathcal{D}_{\nu} \mathbf{Q} \right), \quad \theta = -\frac{\sigma_{\mathrm{xy}}}{8}$ σ_{11}^* n+1 σ_{12}



Zhang, KITP 2008

θ term with open boundaries

• $\theta = \pi$ implies QHE on the boundary with

$$S_{\theta} = \frac{\theta}{2\pi} \frac{\alpha}{16\pi} \int d^3x dt \epsilon_{\mu\nu\rho\tau} F^{\mu\nu} F^{\rho\tau} = \frac{\theta}{2\pi} \frac{\alpha}{4\pi} \int d^3x dt \partial^{\mu} (\epsilon_{\mu\nu\rho\sigma} A^{\nu} \partial^{\rho} A^{\tau})$$

 $\sigma_{xy} = \frac{1}{2} \frac{e^2}{h}$

• For a sample with boundary, it is only insulating when a small T-breaking field is applied to the boundary. The surface theory is a CS term, describing the half QH. • Each Dirac cone contributes $\sigma_{xy}=1/2e^2/h$ to the QH. Therefore, $\theta=\pi$ implies an odd number of Dirac cones on the surface!







• Surface of a TI = 1/4 graphene

The Topological Magneto-Electric (TME) effect

• Equations of axion electrodynamics predict the robust TME effect. Zhang, KITP 2008



• $P_3=\theta/2\pi$ is the electro-magnetic polarization, microscopically given by the CS term over the momentum space. Change of $P_3=2^{nd}$ Chern number!

$$P_{3}(\theta_{0}) = \int d^{3}k\mathcal{K}^{\theta}$$
$$= \frac{1}{16\pi^{2}} \int d^{3}k \epsilon^{\theta i j k} \operatorname{Tr}\left[\left(f_{i j} - \frac{1}{3}[a_{i}, a_{j}]\right) \cdot a_{k}\right]$$

Experimental signature

- Properties of the bulk identifies the topological insulators. Surface states are experimental signature.
- If bulk become conducting, e.g. by doping, surface states seem to disappear.

Is there signature of topological band structure left even in the conducting phase? SC phase, Majorana vortex modes Even appear in some non TI!



Y. Chen, et. Al., Science, **325,** 178

Majorana Modes

- Fermionic mode which is its own anti-particle $C^{-1}\gamma C = \gamma^{\dagger} = \gamma$
- In superconducting states electrons pair: no cost to remove a pair.
- Removing or adding an electron are equivalent.

Vortex in *p+ip* superconductor (Read, Green '00) Semiconductor-ferromagnet-superconductor sandwich (Lutchyn *et. al.* '10) Superconductor-topological insulator interface (Fu, Kane '08)

Majorana modes in TI/SC interface

- Surface Hamiltonian: $H_0 = \psi^{\dagger}(-iv\vec{\sigma}\cdot\nabla-\mu)\psi$
- Associated berry phase of π
- Introduce pairing by proximity effect.

$$\mathcal{H} = -iv\tau^z \sigma \cdot \nabla - \mu\tau^z + \Delta_0(\tau^x \cos\phi + \tau^y \sin\phi)$$
$$\Psi = ((\psi_{\uparrow}, \psi_{\downarrow}), (\psi_{\downarrow}^{\dagger}, -\psi_{\uparrow}^{\dagger}))^T$$



Ghaemi and Wilczek 2007

Fu and Kane 2008



Topological insulator $P(000)P(00\pi) = (+1)(-1) = -1$

Superconducting TIs

- Tis could be doped and be pushed to SC phase. (e.g. Cu doped Bismuth Selenide, *Hor et. Al.* arXiv:1006.0317) *Is there Majorana mode on the edge in the vortex?*
- Large chemical potential: Material does not know about band inversion, lost information about topological features so NO Majorana mode!
- Chemical potential in bulk gap, only pairing on surface, like proximity induced case so Majorana mode.

What happens in between?

First guess!

When surface band cross the bulk band?

If so it would depends on the surface properties.

A single zero modes needs another partner to decay!

Physical picture!

When the transition happens the vortex line becomes gapless. Lets look for the zero energy mode!

In gap states in SC vortices

- Simple s-wave SC vortex (Caroli et. Al. 1964) $E_n \sim (n + \frac{1}{2}) \frac{\Delta^2}{\mu}$
- Experimental observation (Hess et. Al. 1990)

Lattice toy model

• Cubic lattice with *s* and *p* orbitals total spin 1/2

$$S_{+} = s\uparrow, \quad P_{+} = \frac{1}{\sqrt{3}}p_{0}\uparrow - \sqrt{\frac{2}{3}}p_{1}\downarrow, \qquad S_{\pm}(P_{\pm}) \quad \text{even (odd) under inversion}$$
$$TS_{+} = S_{-}, \quad TP_{+} = P_{-},$$
$$S_{-} = s\downarrow, \quad P_{-} = \frac{1}{\sqrt{3}}p_{0}\downarrow + \sqrt{\frac{2}{3}}p_{-1}\uparrow, \qquad TS_{-} = -S_{+}, \quad TP_{-} = -P_{+},$$

$$\mathbb{H} = \Sigma_k \Psi_k^{\dagger} H_k \Psi_k$$

$$\Psi^{\dagger} = (S_+^{\dagger}, S_-^{\dagger}, P_+^{\dagger}, P_-^{\dagger})$$

$$H_k = v_F(\tau_x \sigma_y \sin k_x - \tau_x \sigma_x \sin k_y + \tau_y \sin k_z)$$

$$+ [M + m(\cos k_x + \cos k_y + \cos k_z)]\tau_z$$

$$+ n(\cos k_x + \cos k_y + \cos k_z).$$

 $\mathcal{H}_{\boldsymbol{k}} = v_D \tau_x \boldsymbol{\sigma} \cdot \boldsymbol{k} + (m - \epsilon k^2) \tau_z - \mu$ (Hosur et. Al. 2010)

Numerical approach

Analytical approach

$$\mathcal{H}_{\boldsymbol{k}} = v_D \tau_x \boldsymbol{\sigma} \cdot \boldsymbol{k} + (m - \epsilon k^2) \tau_z - \mu$$

• Add pairing and the vortex, solve for zero energy solution:

$$J(kr) \quad m - \epsilon k^2 = 0 \qquad \mu = \sqrt{m/\epsilon}$$

•This condition is symmetry dependent. What if we don't have circular symmetry?

•Important observation: When $\mu = \sqrt{m/\epsilon}$, Simple Dirac Hamiltonian, Berry phase around the Fermi surface is π

Is this a more general condition?

General Fermi surface criteria

$$\mathcal{H} = \frac{1}{2} \sum_{\boldsymbol{k}\boldsymbol{k}'} \Psi_{\boldsymbol{k}}^{\dagger} \mathcal{H}^{\text{BdG}}(\boldsymbol{k}, \boldsymbol{k}') \Psi_{\boldsymbol{k}'} \qquad \qquad \mathcal{H}^{\text{BdG}} = \begin{bmatrix} H_{\boldsymbol{k}} - \mu & \Delta(\boldsymbol{r}) \\ \Delta^{*}(\boldsymbol{r}) & \mu - H_{\boldsymbol{k}} \end{bmatrix}$$

$$\Delta(r) = \frac{\Delta_0}{\xi}(x - iy)$$

$$\mathcal{H}_{\boldsymbol{k}}^{\mathrm{BdG}} = \begin{bmatrix} H_{\boldsymbol{k}} - \mu & i\frac{\Delta_0}{\xi}(\partial_{k_x} - i\partial_{k_y}) \\ i\frac{\Delta_0}{\xi}(\partial_{k_x} + i\partial_{k_y}) & \mu - H_{\boldsymbol{k}} \end{bmatrix} \qquad \qquad H_{\boldsymbol{k}}|\varphi_{\boldsymbol{k}}\rangle = E|\varphi_{\boldsymbol{k}}\rangle$$

$$\tilde{\mathcal{H}}_{\boldsymbol{k}}^{\mathrm{BdG}} = \begin{bmatrix} E_{\boldsymbol{k}} - \mu & i\frac{\Delta_0}{\xi}(D_{k_x} - iD_{k_y}) \\ i\frac{\Delta_0}{\xi}(D_{k_x} + iD_{k_y}) & -E_{\boldsymbol{k}} + \mu \end{bmatrix}$$

Inversion Symmetry! Degenerate FS

 $D_{k_{\alpha}} = \partial_{k_{\alpha}} - i\mathbf{A}_{\alpha}(\mathbf{k}) \qquad [\mathbf{A}]^{\mu\nu}_{\alpha}(\mathbf{k}) = i\langle\varphi^{\mu}_{\mathbf{k}}|\partial_{k_{\alpha}}|\varphi^{\nu}_{\mathbf{k}}\rangle$

Zero energy states

$$\tilde{\mathcal{H}}_{\boldsymbol{k}}^{\text{BdG}} = \begin{bmatrix} E_{\boldsymbol{k}} - \mu & i\frac{\Delta_0}{\xi}(D_{k_x} - iD_{k_y}) \\ i\frac{\Delta_0}{\xi}(D_{k_x} + iD_{k_y}) & -E_{\boldsymbol{k}} + \mu \end{bmatrix}$$

 $D_{k_{\alpha}} = \partial_{k_{\alpha}} - i\mathbf{A}_{\alpha}(\mathbf{k}) \qquad [\mathbf{A}]^{\mu\nu}_{\alpha}(\mathbf{k}) = i\langle \varphi^{\mu}_{\mathbf{k}} | \partial_{k_{\alpha}} | \varphi^{\nu}_{\mathbf{k}} \rangle$

Diagonal $[\mathbf{A}]^{\mu\nu}_{\alpha}$ two copies of P+iP. But with finite size (FS size) in momentum space: Finite size effect $\mathcal{O}(\frac{\Delta_0}{k_F\xi})$

Effect of gauge potential phase of

$$U = e^{i \oint \mathbf{A}.d\mathbf{l}}$$

Nonabelian Berry phase!

Semiclassical Bohr-Sommerfield quantization:

$$E_n = \frac{\Delta_0}{l_F \xi} (2\pi n + \pi \pm \phi_B)$$

Candidate Materials

- Among doped topological insulators:
 - p-doped TlBiTe₂
 - *p*-doped Bi_2Te_3 under pressure
 - *n*-doped Bi_2Te_3
 - not *n*-doped Bi_2Se_3
- Among ordinary insulators
 - Either PbTe or SnTe and GeTe (PbTe has four band inversions relative to SnTe and GeTe)

Summary

- Majorana fermion states can appear as single zero energy states in superconductors owing to their builtin particle-hole symmetry
- Several examples exist in model systems, but none of them have been realized in experiment so far.
- We find that a superconductor whose parent compound is a topological insulator will host Majorana modes at the ends of a vortex if the doping is not too high, and find real material examples.
- The general theory allows non-topological insulatorbased superconductors to host Majorana modes as well