## **Topological Band Theory III**

- I. Topological Insulators in 3D
  - Weak vs strong

Lecture notes available at https://www.lorentz.leidenuniv.nl/lorentzchair/

- Topological invariants from band structure
- II. The surface of a topological insulator
  - Quantum Hall effect
  - $\boldsymbol{\theta}$  term and topological magnetoelectric effect
  - Superconductivity
  - Surface topological order
- III. Topological Superconductivity
  - 1D topological superconductor
  - Majorana chain
  - 2D topological superconductor
  - 10-fold way
  - Majorana modes and quantum information

Next Week same time, same place : Topological Mechanics

## **3D** Topological Insulators

There are 4 surface **Dirac Points** due to Kramers degeneracy







Surface Brillouin Zone

 $k=\Lambda_a$   $k=\Lambda_b$   $k=\Lambda_a$   $k=\Lambda_b$ How do the Dirac points connect? Determined by 4 bulk Z<sub>2</sub> topological invariants v<sub>0</sub>; (v<sub>1</sub>v<sub>2</sub>v<sub>3</sub>)

 $v_0 = 0$ : Weak Topological Insulator

Related to layered 2D QSHI ;  $(v_1v_2v_3) \sim$  Miller indices Fermi surface encloses even number of Dirac points

 $v_0 = 1$ : Strong Topological Insulator

Fermi circle encloses odd number of Dirac points Topological Metal :

1/4 graphene Berry's phase  $\pi$ Robust to disorder: impossible to localize



 $Bi_{1-x}Sb_x$ 

Theory: Predict  $Bi_{1-x}Sb_x$  is a topological insulator by exploiting inversion symmetry of pure Bi, Sb (Fu,Kane PRL'07)

Experiment: ARPES (Hsieh et al. Nature '08)



- Bi<sub>1-x</sub> Sb<sub>x</sub> is a Strong Topological Insulator  $v_0$ ;  $(v_1, v_2, v_3) = 1$ ; (111)
- 5 surface state bands cross E<sub>F</sub> between  $\Gamma$  and M

 $Bi_2 Se_3$ 



exposing to  $NO_2$ 

Band Theory :

ARPES Experiment : Y. Xia et al., Nature Phys. (2009). H. Zhang et. al, Nature Phys. (2009).

- $v_0;(v_1,v_2,v_3) = 1;(000)$  : Band inversion at  $\Gamma$
- Energy gap:  $\Delta \sim .3 \text{ eV}$  : A room temperature topological insulator
- Simple surface state structure : Similar to graphene, except only a single Dirac point



## **Topological Invariants in 3D**

1.  $2D \rightarrow 3D$ : Time reversal invariant planes

The 2D invariant

$$(-1)^{\nu} = \prod_{a=1}^{4} \delta(\Lambda_a) \qquad \delta(\Lambda_a) = \frac{\Pr[w(\Lambda_a)]}{\sqrt{\det[w(\Lambda_a)]}}$$

Each of the time reversal invariant planes in the 3D Brillouin zone is characterized by a 2D invariant.

Weak Topological Invariants (vector):

$$(-1)^{\nu_i} = \prod_{a=1}^4 \delta(\Lambda_a) \Big|_{\substack{k_i=0\\plane}} \qquad \mathbf{G}_{\nu} = \frac{2\pi}{a} (\nu_1, \nu_2, \nu_3)$$

"mod 2" reciprocal lattice vector indexes lattice planes for layered 2D QSHI

Strong Topological Invariant (scalar)

$$(-1)^{\nu_o} = \prod_{a=1}^8 \delta(\Lambda_a)$$



## **Topological Invariants in 3D**

#### 2. $4D \rightarrow 3D$ : Dimensional Reduction

Add an extra parameter,  $k_4$ , that smoothly connects the topological insulator to a trivial insulator (while breaking time reversal symmetry)



n depends on how  $H(\mathbf{k})$  is connected to  $H_0$ , but due to time reversal, the difference must be even.

 $v_0 = n \mod 2$ 

Express in terms of Chern Simons 3-form :  $Tr[F \wedge F] = dQ_3$ 

$$v_0 = \frac{1}{4\pi^2} \int d^3 k Q_3(\mathbf{k}) \mod 2 \qquad \qquad Q_3(\mathbf{k}) = \operatorname{Tr}[\mathbf{A} \wedge d\mathbf{A} + \frac{2}{3}\mathbf{A} \wedge \mathbf{A} \wedge \mathbf{A}]$$

Gauge invariant up to an even integer.

Unique Properties of Topological Insulator Surface States



Broken symmetry (or strong interactions) leads to exotic gapped states

- Quantum Hall state, topological magnetoelectric effect Fu, Kane '07; Qi, Hughes, Zhang '08, Essin, Moore, Vanderbilt '09
- Superconducting state
   Fu, Kane '08
- Surface topological order: symmetry preserving gapped state Metlitski, Kane, Fisher '13, Bonderson, Nayak, Qi '13, Chen, Fidkowski, Vishwanath '13, Wang, Potter, Senthil '14

## Surface Quantum Hall Effect

Orbital QHE : E=0 Landau Level for Dirac fermions. "Fractional" IQHE



Anomalous QHE : Induce a surface gap by depositing magnetic material

$$H_0 = \psi^{\dagger} (-i v \vec{\sigma} \cdot \vec{\nabla} - \mu + \Delta_M \sigma_z) \psi$$

 $^{\uparrow}\mathsf{E}_{\mathsf{gap}} = 2|\Delta_{\mathsf{M}}|$ 

E<sub>F</sub>

Mass due to Exchange field

$$\sigma_{xy} = \operatorname{sgn}(\Delta_M) \frac{e^2}{2h}$$



Chiral Edge State at Domain Wall :  $\Delta_{M} \leftrightarrow -\Delta_{M}$ 

### **Topological Magnetoelectric Effect**

Qi, Hughes, Zhang '08; Essin, Moore, Vanderbilt '09

Consider a solid cylinder of TI with a magnetically gapped surface

$$J = \sigma_{xy}E = \frac{e^2}{h}\left(n + \frac{1}{2}\right)E = M$$

Magnetoelectric Polarizability

$$M = \alpha E \quad \alpha = \frac{e^2}{h} \left( n + \frac{1}{2} \right)$$

topological " $\theta$  term"  $\Delta L = \alpha \mathbf{E} \cdot \mathbf{B}$   $\alpha = \theta \frac{e^2}{2\pi h}$ 

TR sym. :  $\theta = 0$  or  $\pi \mod 2\pi$ 

The fractional part of the magnetoelectric polarizability is determined by the bulk, and independent of the surface (provided there is a gap) Analogous to the electric polarization, P, in 1D.

Ε

 $d=1: Polarization P \qquad P \cdot E \qquad \frac{e}{2\pi} \int_{BZ} Tr[A] \qquad e \qquad (extra end electron) \\ d=3: Magnetoelectric poliarizability \alpha \qquad \alpha E \cdot B \qquad \frac{e^2}{4\pi^2 h} \int_{BZ} Tr[A \wedge dA + \frac{2}{3}A \wedge A \wedge A] \qquad e^2 / h \qquad (extra surface quantum Hall layer) \\ \end{array}$ 

### Superconducting proximity effect on a topological insulator

Proximity to superconductor introduces energy gap by breaking gauge symmetry

$$H = \psi^{\dagger} (-i v \vec{\sigma} \cdot \vec{\nabla} - \mu) \psi$$
$$+ \Delta_{S} \psi^{\dagger} \psi^{\dagger} + \Delta_{S}^{*} \psi_{\downarrow} \psi_{\uparrow}$$



- Half an ordinary superconductor
- Similar to spinless  $p_x + ip_y$  superconductor, except :
  - Does not violate time reversal symmetry
  - s-wave singlet superconductivity
  - Required minus sign is provided by  $\pi$  Berry's phase due to Dirac Point
- Nontrivial ground state supports Majorana fermion bound states at vortices



# **Strong Interactions**

Topological Insulator coupled to compact U(1) gauge field, A

For a compact gauge field, magnetic monopoles are excitations in the theory. Useful diagnostic for strongly interacting theories.

Low energy theory for A :  $\theta$  term

Qi, Hughes and Zhang '08

$$S = i\theta N \qquad \qquad N = \frac{1}{32\pi^2} \int d^3x d\tau \varepsilon_{\mu\nu\lambda\rho} F_{\mu\nu} F_{\lambda\rho} \in \mathbb{Z}$$

- Time reversal symmetry :  $\theta = 0$  or  $\pi \mod 2\pi$ .  $\theta = \pi \mod 2\pi$  for electron TI
- Witten Effect: Magnetic monopoles are charged  $Q = \frac{\theta}{2\pi}e$
- Monopoles (or dyons) are bosons with half integer charge  $Q = e\left(n + \frac{1}{2}\right)$

#### Can the surface of a TI be gapped without breaking symmetry ?

Pass monopole from inside to outside of TI :



Break T at surface:

 $\sigma_{xy} = e^2/2h$ : charge e/2 flows away on surface

Superconductor at surface:

Charge conservation is violated at surface

Keep U(1) and T at surface :

Charge e/2 stays at surface :

Requires a topologically ordered surface state with e/2 quasiparticle

#### Requirements for a Topological Surface Phase on fermion TI

It should be impossible in 2D if symmetry is preserved, but if symmetry is broken there should be a 2D state with the same topological order



Broken T: Topo – M slab



A 2D Non-Abelian quantum Hall state with

- Hall conductance  $v e^2/h$ ; v = 1/2
- Thermal Hall cond.  $c \pi^2 k_B^2/6h$ ; c = 1/2



Theories of symmetry preserving gapped state:

Related to Moore-Read (Pfaffian) state of FQHE at v=1/2

- "T-Pfaffian state" Bonderson, Nayak, Qi '13; Chen, Fidkowski, Vishwanath '13
- "Moore-Read/antisemion state" Metlitski, Kane, Fisher '13 ; Wang, Potter, Senthil '13

### **BCS** Theory of Superconductivity

mean field theory: 
$$\Psi^{\dagger}\Psi\Psi^{\dagger}\Psi \Rightarrow \langle \Psi^{\dagger}\Psi^{\dagger}\rangle\Psi\Psi = \Delta^{*}\Psi\Psi$$
  
 $H = \frac{1}{2}\sum_{\mathbf{k}} (\Psi^{\dagger} \quad \Psi)H_{BdG} \begin{pmatrix} \Psi\\ \Psi^{\dagger} \end{pmatrix} \qquad \begin{array}{c} \text{Bogoliubov de Gennes}\\ \text{Hamiltonian} \end{array} \qquad H_{BdG} = \begin{pmatrix} H_{0} & \Delta\\ \Delta^{*} & -H_{0} \end{pmatrix}$ 

Intrinsic anti-unitary particle – hole symmetry

$$\varphi_{-E} = \Xi \varphi_{E} \implies \gamma_{E}^{\dagger} = \gamma_{-E}$$

Bloch - BdG Hamiltonians satisfy  $\Xi H_{BdG}(\mathbf{k})\Xi^{-1} = -H_{BdG}(-\mathbf{k})$ Topological classification problem similar to time reversal symmetry 1D  $\mathbb{Z}_2$  Topological Superconductor : v = 0,1 (Kitaev, 2000)

Bulk-Boundary correspondence : Discrete end state spectrum **END**  $\nu=0$  "trivial" "topological"  $\nu = 1$ Ε Zero mode  $\Delta$  $\Delta$ Ε  $\Gamma^{\dagger}_{E=0}$  $\equiv \gamma$ E=0 $=\Gamma_{E=0}$ 0  $\mathbf{0}$ -E  $\Gamma_{-F} = \Gamma^{\dagger}_{F}$ Majorana fermion  $-\Delta$  $-\Delta$ bound state

Majorana Fermion : Particle = Antiparticle  $\gamma = \gamma^{\dagger}$ 

Real part of a Dirac fermion : 
$$\begin{cases} \gamma_1 = \Psi + \Psi^{\dagger} & ; \quad \Psi = \gamma_1 + i\gamma_2 & \gamma_i^2 = 1\\ \gamma_2 = -i(\Psi - \Psi^{\dagger}) & ; \quad \Psi^{\dagger} = \gamma_1 - i\gamma_2 & \left\{\gamma_i, \gamma_j\right\} = 2\delta_{ij} \end{cases}$$

"Half a state"

Two Majorana fermions define a single two level system

$$H = 2i\varepsilon_0\gamma_1\gamma_2 = \varepsilon_0\Psi^{\dagger}\Psi$$



#### Kitaev Model for 1D p wave superconductor

$$H_{BdG}(k) = \tau_z (2t\cos k - \mu) + \tau_x \Delta \sin k = \mathbf{d}(k) \cdot \overline{\tau}$$

|μ|>2t : Strong pairing phase trivial superconductor

|μ|<2t : Weak pairing phase topological superconductor



Similar to SSH model, except different symmetry :  $(d_x, d_y, d_z)\Big|_{k} = (-d_x, -d_y, d_z)\Big|_{k}$ 

## Majorana Chain

$$c_i \rightarrow \gamma_{1i} + i\gamma_{2i} \qquad H = 2i\sum_i t_1\gamma_{1i}\gamma_{2i} + t_2\gamma_{2i}\gamma_{1i+1}$$

 $\mu c_i^{\dagger} c_i \rightarrow 2i \mu \gamma_{1i} \gamma_{2i}$   $t \left( c_i^{\dagger} c_{i+1} + c_{i+1}^{\dagger} c_i \right) \rightarrow 2it \left( \gamma_{1i} \gamma_{2i+1} - \gamma_{2i} \gamma_{1i+1} \right)$   $\Delta \left( c_i c_{i+1} + c_{i+1}^{\dagger} c_i^{\dagger} \right) \rightarrow 2i \Delta \left( \gamma_{1i} \gamma_{2i+1} + \gamma_{2i} \gamma_{1i+1} \right)$ 

For  $\Delta$ =t : nearest neighbor Majorana chain

$$t_1 = \mu, \ t_2 = 2t$$



#### $2D \mathbb{Z}$ topological superconductor (broken T symmetry)

Bulk-Boundary correspondence:

n = # Chiral Majorana Fermion edge states





Read Green model : 
$$H = \sum_{\mathbf{k}} \left( \frac{\mathbf{k}^2}{2m} - \mu \right) c_{\mathbf{k}}^{\dagger} c_{\mathbf{k}} + (\Delta(\mathbf{k})c_{\mathbf{k}}c_{-\mathbf{k}} + c.c.)$$
  $\Delta(\mathbf{k}) = \Delta_0 \left( k_x + ik_y \right)$   
Lattice BdG model :  $H_{BdG}(\mathbf{k}) = \tau_z \left( 2t \left[ \cos k_x + \cos k_y \right] - \mu \right) + \Delta \left( \tau_x \sin k_x + \tau_y \sin k_y \right) = \mathbf{d}(k) \cdot \vec{\tau}$   
 $|\mu| > 4t$  : Strong pairing phase  
trivial superconductor  $d_y$   $d(\mathbf{k})$  Chern number 0  
 $|\mu| < 4t$  : Weak pairing phase  
topological superconductor  $d_y$  Chern number 1

#### Periodic Table of Topological Insulators and Superconductors

Anti-Unitary Symmetries :

- Time Reversal :  $\Theta H(\mathbf{k})\Theta^{-1} = +H(-\mathbf{k}); \quad \Theta^2 = \pm 1$
- $\Xi H(\mathbf{k})\Xi^{-1} = -H(-\mathbf{k}); \quad \Xi^2 = \pm 1$ - Particle - Hole :

 $\Pi H(\mathbf{k})\Pi^{-1} = -H(\mathbf{k}) ; \quad \Pi \propto \Theta \Xi$ Unitary (chiral) symmetry :



<sup>8</sup> antiunitary symmetry classes

		Symmetry				d								
Altland- Zirnbauer Random Matrix Classes		AZ	Θ	Ξ	Π	1	2	3	4	5	6	$\overline{7}$	8	
	$\left( \right)$	А	0	0	0	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	Complex
		AIII	0	0	1	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	∫ K-theory
		AI	1	0	0	0	0	0	$\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	
		BDI	1	1	1	$\mathbb{Z}$	0	0	0	$\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	
		D	0	1	0	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$\mathbb{Z}$	0	$\mathbb{Z}_2$	
		DIII	-1	1	1	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$\mathbb{Z}$	0	Real
		AII	-1	0	0	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$\mathbb{Z}$	(K-theory
		CII	-1	-1	1	$\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	
		$\mathbf{C}$	0	-1	0	0	$\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	
		CI	1	-1	1	0	0	$\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	)
<i></i>	Ľ													

Kitaev, 2008 Schnyder, Ryu, Furusaki, Ludwig 2008

Bott Periodicity  $d \rightarrow d+8$ 

### Majorana zero mode at a vortex



Boundary condition on fermion wavefunction

$$\psi(L) = (-1)^{p+1} \psi(0)$$

$$\psi(x) \propto e^{iq_m x}$$
;  $q_m = \frac{\pi}{L} (2m+1+p)$ 

Hole in a topological superconductor threaded by flux



Without the hole : Caroli, de Gennes, Matricon theory ('64)

### Majorana Bound States on Topological Insulators



Quasiparticle Bound state at E=0



Majorana Fermion  $\gamma_0$  "Half a State"

2. Superconductor-magnet interface at edge of 2D QSHI





Domain wall bound state  $\gamma_0$ 

### 1D Majorana Fermions on Topological Insulators

1. 1D Chiral Majorana mode at superconductor-magnet interface



Gapless non-chiral Majorana fermion for phase difference  $\phi = \pi$  $H = -i\hbar V_{F} \left( \gamma_{L}\partial_{x}\gamma_{L} - \gamma_{R}\partial_{x}\gamma_{R} \right) + i\Delta\cos(\phi/2)\gamma_{L}\gamma_{R}$ 

### Majorana Fermions and Topological Quantum Computing

(Kitaev '03)

The degenerate states associated with Majorana zero modes define a topologically protected quantum memory

- 2 Majorana separated bound states = 1 fermion  $\Psi = \gamma_1 + i\gamma_2$ 
  - 2 degenerate states (full/empty) = 1 qubit
- 2N separated Majoranas = N qubits
- Quantum Information is stored non locally
  - Immune from local decoherence

Braiding performs unitary operations Non-Abelian statistics

Interchange rule (Ivanov 03)

$$\begin{array}{c} \gamma_i \to \gamma_j \\ \gamma_j \to -\gamma_i \end{array}$$

These operations, however, are not sufficient to make a universal quantum computer



Potential condensed matter hosts for Majorana modes

- Quasiparticles in fractional Quantum Hall effect at v=5/2 Moore Read '91
- Unconventional superconductors
  - Sr<sub>2</sub>RuO<sub>4</sub> Das Sarma, Nayak, Tewari '06
  - Fermionic atoms near feshbach resonance Gurarie '05
  - Cu<sub>x</sub>Bi<sub>2</sub>Se<sub>3</sub> ?
- Proximity Effect Devices using ordinary superconductors
  - Topological Insulator devices Fu, Kane '08
  - 2D Semiconductor/Magnet devices Sau, Lutchyn, Tewari, Das Sarma '09, Lee '09
  - 1D Semiconductor devices: eg In As quantum wires
     Expt :
     Oreg, von Oppen, Alicea, Fisher '10 Lutchyn, Sau, Das Sarma '10 Maurik et al. (Kouwenhoven) '12
  - 1D Ferromagnetic atomic chains on superconductors Expt : Nadj-Perg et al. (Yazdani) '14