



K理論とトポロジカル結晶物質

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Outline

- 1. Topological (crystalline) insulators/superconductors
- 2. K-group classification
- 3. Nonsymmorphic symmetry and new topological phases

Mobius twisted surface states

Shiozaki-MS, Phys. Rev. B90, 166114 (2014). [41pages] Shiozaki-MS-Gomi, Phys. Rev. B91, 155120 (2015). Shiozaki-MS-Gomi, Phys. Rev. B93, 195413 (2016). Shiozaki-MS-Gomi, Phys. Rev. B95, 235425 (2017). [Editor's suggestion, 54pages]

Introduction

The idea of topological insulator/superconductor (TI/TSC) has been successfully established with many experimental supports for surface states

TI/TSC = Non-trivial topological # of occupied state



The non-trivial topological structure predicts the existence of gapless surface states



TIs/TSCs have gapless boundary states ensured by bulk topological numbers

bulk-boundary correspondence 4

Topological insulator (TI)

insulator supporting surface Dirac fermions



Topological SCs

spin-triplet (odd-parity) SC [MS (09, 10), Fu-Berg (10)]



Cu_xBi₂Se₃



Experiment

[Sasaki-Kriener-Segawa-Yada-Tanaka-MS – Ando (11)]

Theory

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[Yamakage-Yada-MS-Tanaka (12)]

S-wave SCs can host topological superconductivity if a spinless system is realized effectively

• Dirac fermion + s-wave condensate

$$\mathcal{H} = \left(\begin{array}{cc} -i\sigma_i\partial_i & \Phi^* \\ \Phi & i\sigma_i\partial_i \end{array} \right)$$

MS(03)

Fu-Kane (08)



• S-wave superconducting state with Rashba SO + Zeeman field



1D Nanowire Lutchyn et al (10), Oreg et al (10) nanowire Zeeman field MF 400 (2e²/h) Mourik *et al.*, Science (2012) 0.3 200 ν (μV) 0 0.2 -200 0.1 InSb/ **NbTiN** -0.25 0.25 0.5 0.75 0 *B* (T)

Majorana Fermion

[MS-Takahashi-Fujimoto (09), J. Sau et al (10)]

Key to realize TI/TSC = Symmetry

Time-reversal symmetry (TRS)



Kramers pair

IUHS

- No back scattering
- topologically stable

Particle-hole symmetry (PHS)

● ≈ ○ + \

Majorana fermion

[StotmoydseiRerusFinious #83] Judwig (12)]

		TRS	PHS	CS	d=1	d=2	d=3		
	А	0	0	0	0	Z	0	Majorana nanowire	
	AIII	0	0	1	Z	0	Z	nuin chiral n	
	AI	1	0	0	0	0	0	p+p chiral p Sr ₂ RuO, ³ He-A	
	BDI	1	1	1	Z	0	0		
	D	0	1	0	(Z_2)	(Z) <	0		
	DIII	-1	1	1	Z ₂	Z_2	Z	³ He-B	
	All	-1	0	0	0	(Z_2)	(Z_2)		
	CII	-1	-1	1	2Z	U	Z ₂	Cu Bi Se	
	C	0	-1	0	0	2Z	0		
	CI	1	-1	1	0	0	2Z		
								QSH 9	

Topological Crystalline Insulator [L. Fu (11), Hsieh et al (12)]

Recently, it has been recognized that point group symmetry also provides novel topological surface states



Idea

Using the eigen value of mirror operator, ky=0 plane can be separated into two QH states.



Topological Crystalline superconductor [Ueno-MS et al (13), Zhang-Kane-Mele (13))



mirror reflection symmetry \mathcal{M}_{xy}

$$(x, y, z) \rightarrow (x, y, -z)$$

 $(\sigma_x, \sigma_y, \sigma_z) \rightarrow (-\sigma_x, -\sigma_y, \sigma_z)$



$$\mathcal{M}_{xy}\mathcal{H}(k_x,k_y,k_z)\mathcal{M}_{xy}^{-1} = \mathcal{H}(k_x,k_y,-k_z)$$
$$[\mathcal{M}_{xy},\mathcal{H}(k_x,k_y,0)] = 0$$

Application to Sr₂RuO₄

[Ueno-MS et al (13)]



In the presence of magnetic fields along the z-direction, NMR date suggests

$$\mathcal{M}_{xy}\Delta(k_x,k_y,k_z)\mathcal{M}_{xy}^t = -\Delta(k_x,k_y,-k_z)$$

We can expect Majorana Fermions !!



Questions

- Is it possible to classify such topological phases systematically?
- How many new topological phases can we obtain in the presence of additional symmetry?

To answer these questions, we employ the K-theory.

Shiozaki-MS, Phys. Rev. B90, 166114 (2014). Shiozaki-MS-Gomi, Phys. Rev. B91, 155120 (2015). Shiozaki-MS-Gomi, arXiv:1511.01463.

Our setting

In stead of occupied states, we classify flattened Hamiltonians



The flattened Hamiltonian defines a map from momentum space to Hilbert space



If the map defines a non-trivial homotopy, we may have a nontrivial topological phase Why we use K-theory?

Adding topologically trivial bands makes the classification simpler

[Kitaev(09)]

In addition to simple deformation of Hamiltonians, the Ktheory approach allows us to add topologically trivial bands during the deformation of Hamiltonians

stable equivalence $\mathcal{H}_1 \simeq \mathcal{H}_2$

deformable by adding extra trivial bands



The stable-equivalence classes defines topological phases

Importantly, using stable equivalence, we can avoid annoying interference between topological charges



Classification of TCIs and TCSCs: K-theory approach

In general, topological phases can be understood as the existence of topological objects in the momentum space



2 dim top. phase



2dim BZ = 2dim torus

"monopole"

Chern number

$$Ch_{1} = \int_{2dBZ} \left(\frac{dS}{2\pi} \right) \cdot \left[\boldsymbol{\nabla} \times \mathcal{A}(\boldsymbol{k}) \right]$$

$$A(\boldsymbol{k}) = i \sum_{\boldsymbol{\lambda}} \left[\langle \boldsymbol{u}, (\boldsymbol{k}) \rangle \right] \boldsymbol{\nabla} \langle \boldsymbol{u}, (\boldsymbol{k}) \rangle$$

$$\mathcal{A}(m{k}) = i \sum_{n \in ext{occ}} \langle u_n(m{k}) | m{
abla} u_n(m{k})
angle$$
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In the framework of K-theory, one can increase the dimension of the system systematically Teo-Kane (10)

$$H_{d+1}(\boldsymbol{k}, k_{d+1}) = \begin{cases} H_d(\boldsymbol{k}) \cos k_{d+1} + \Gamma \sin k_{d+1} & \text{chiral case} \\ (H_d(\boldsymbol{k}) \otimes \sigma_z) \cos k_{d+1} + (1 \otimes \sigma_y) \sin k_{d+1} & \text{non-chiral case} \end{cases}$$



This map keeps the topological number but it shifts the symmetry of the system

class DIII (TRI SCs)										
$CH_d(\mathbf{k})C^{-1} = -H$	$H_d(-oldsymbol{k})$	C	$\tau = \tau_x K$	ζ ($C^{2} = 1$					
$TH_d(\mathbf{k})T^{-1} = H_d$	$(-oldsymbol{k})$	Т	$= i s_y I$	K T	$y^2 = -1$					
$H_{d+1}(\boldsymbol{k}, k_{d+1}) = H_d(\boldsymbol{k}) \cos k_{d+1} + \Gamma \sin k_{d+1} \Gamma = iTC$										
class All (TRI Insulators) This term										
$TH_{d+1}(\boldsymbol{k}, k_{d+1})T^{-}$	br	eaks Pl	HS							
		TRS	PHS	CS	d=1	d=2	d=3			
	AI	1	0	0	0	0	0			
	BDI	1	1	1	Z	0	0			
	D	0	1	0	Z_2		0			
hierarchy of top #	DIII	-1	1	1	Ζ,	Z,	<u> </u>			
	All	-1	0	0	0	Ζ,	Z ₂			
	CII	-1	-1	1	2Z	0	Ζ ₂			
	С	0	-1	0	0	2Z	0			
	CI	1	-1	1	0	0	22	21		

We generalize this idea to systems with additional symmetry

Shiozaki-MS(14)

class DIII (TRI SCs) + mirror reflection

$$\begin{array}{ll} CH_{d}(\boldsymbol{k})C^{-1} = -H_{d}(-\boldsymbol{k}) & C = \tau_{x}K & C^{2} = 1 \\ TH_{d}(\boldsymbol{k})T^{-1} = H_{d}(-\boldsymbol{k}) & T = is_{y}K & T^{2} = -1 \\ UH_{d}(\boldsymbol{k})U^{-1} = H_{d}(-k_{1},k_{2},\ldots,k_{d}) & U = is_{x} \end{array}$$

$$H_{d+1}(\boldsymbol{k}, k_{d+1}) = H_d(\boldsymbol{k}) \cos k_{d+1} + \Gamma \sin k_{d+1} \quad \Gamma = iTC$$

This term keeps mirror sym.

class All (TRI Insulators) + mirror reflection

$$TH_{d+1}(\mathbf{k}, k_{d+1})T^{-1} = H_{d+1}(-\mathbf{k}, -k_{d+1})$$
$$UH_{d+1}(\mathbf{k})U^{-1} = H_{d+1}(-k_1, k_2, \dots, k_d, k_{d+1})$$
mirror sym.

However, this is not the only possibility

The mapped Hamiltonian also has a different additional symmetry



In this manner, we can change the number of flipped coordinates d_{||} under the symmetry, with keeping the topological structure



Using these relations, we complete the classification of TCIs and TCSCs protected by order-two space (and magnetic space) groups

Extended topological Table

A single periodic table with 10 different topological class

[Schnyder et al (08)]

6 periodic tables with 27 classes +6 periodic tables with 10 classes

[Shiozaki-MS (14),

Shiozaki-MS-Gomi (15)]

		Symmetry	Class	\mathcal{C}_q or \mathcal{R}_q	$\delta = 0$	$\delta = 1$	$\delta = 2$	$\delta = 3$	$\delta = 4$	$\delta = 5$	$\delta = 6$	$\delta = 7$
Sr ₂ RuO ₄		U	А	\mathcal{C}_1	0	\mathbb{Z}	0	\mathbb{Z}	0	\mathbb{Z}	0	\mathbb{Z}
	Lange to the 1916 of the	U_+	AIII	C_0	\mathbb{Z}	0	\mathbb{Z}	0	\mathbb{Z}	0	\mathbb{Z}	0
** **	0.12 - probability	U_{-}	AIII	$\mathcal{C}_1 imes \mathcal{C}_1$	0	$\mathbb{Z}\oplus\mathbb{Z}$	0	$\mathbb{Z}\oplus\mathbb{Z}$	0	$\mathbb{Z}\oplus\mathbb{Z}$	0	$\mathbb{Z}\oplus\mathbb{Z}$
	0.08 –		AI	\mathcal{R}_1	\mathbb{Z}_2	\mathbb{Z}	0	0	0	$2\mathbb{Z}$	0	\mathbb{Z}_2
Sr J	0.04 -		BDI	\mathcal{R}_2	\mathbb{Z}_2	\mathbb{Z}_2	\mathbb{Z}	0	0	0	$2\mathbb{Z}$	0
)	D	\mathcal{R}_3	-0	\mathbb{Z}_2	\mathbb{Z}_2	\mathbb{Z}	0	0	0	$2\mathbb{Z}$
Ru	x ¹⁵ + ¹⁵ y	$U_{+}^{+}, U_{-}^{-}, U_{++}^{+}, U_{}^{-}$	DIII	\mathcal{R}_4	$2\mathbb{Z}$	0	\mathbb{Z}_2	\mathbb{Z}_2	\mathbb{Z}	0	0	0
0			AII	\mathcal{R}_5	0	$2\mathbb{Z}$	0	\mathbb{Z}_2	\mathbb{Z}_2	\mathbb{Z}	0	0
			CII	\mathcal{R}_6	0	0	$2\mathbb{Z}$	0	\mathbb{Z}_2	\mathbb{Z}_2	\mathbb{Z}	0
			\mathbf{C}	\mathcal{R}_7	0	0	0	$2\mathbb{Z}$	0	\mathbb{Z}_2	\mathbb{Z}_2	\mathbb{Z}
			CI	\mathcal{R}_0	\mathbb{Z}	0	0	0	$2\mathbb{Z}$	0	\mathbb{Z}_2	\mathbb{Z}_2
		U^+_{+-}, U^{-+}	BDI	$\mathcal{R}_1 \times \mathcal{R}_1$	$\mathbb{Z}_2 \oplus \mathbb{Z}_2$	$\mathbb{Z}\oplus\mathbb{Z}$	0	0	0	$2\mathbb{Z}\oplus 2\mathbb{Z}$	0	$\mathbb{Z}_2 \oplus \mathbb{Z}_2$
		U^+_{-+}, U^{+-}	DIII	$\mathcal{R}_3 imes \mathcal{R}_3$	0	$\mathbb{Z}_2 \oplus \mathbb{Z}_2$	$\mathbb{Z}_2 \oplus \mathbb{Z}_2$	$\mathbb{Z}\oplus\mathbb{Z}$	0	0	0	$2\mathbb{Z}\oplus 2\mathbb{Z}$
		U^+_{+-}, U^{-+}	CII	$\mathcal{R}_5 imes \mathcal{R}_5$	0	$2\mathbb{Z}\oplus 2\mathbb{Z}$	0	$\mathbb{Z}_2 \oplus \mathbb{Z}_2$	$\mathbb{Z}_2 \oplus \mathbb{Z}_2$	$\mathbb{Z}\oplus\mathbb{Z}$	0	0
a -		U^+_{-+}, U^{+-}	CI	$\mathcal{R}_7 imes \mathcal{R}_7$	0	0	0	$2\mathbb{Z}\oplus 2\mathbb{Z}$	0	$\mathbb{Z}_2 \oplus \mathbb{Z}_2$	$\mathbb{Z}_2 \oplus \mathbb{Z}_2$	$\mathbb{Z}\oplus\mathbb{Z}$
SnTe			AI	\mathcal{R}_7	0	0	0	$2\mathbb{Z}$	0	\mathbb{Z}_2	\mathbb{Z}_2	\mathbb{Z}
			BDI	\mathcal{R}_0	\mathbb{Z}	0	0	0	$2\mathbb{Z}$	0	\mathbb{Z}_2	\mathbb{Z}_2
			D	\mathcal{R}_1	\mathbb{Z}_2	\mathbb{Z}	0	0	0	$2\mathbb{Z}$	0	\mathbb{Z}_2
Sn - TR		$U_{-}^{+}, U_{+}^{-}, U_{}^{+}, U_{++}^{-}$	DIII	\mathcal{R}_2	\mathbb{Z}_2	\mathbb{Z}_2	\mathbb{Z}		0	0	$2\mathbb{Z}$	0
THIT			AII	\mathcal{R}_3	0	\mathbb{Z}_2		\mathbb{Z}	0	0	0	$2\mathbb{Z}$
	$\frac{1}{9}$ <i>hv</i> = 21.2 eV		CII	\mathcal{R}_4	$2\mathbb{Z}$	0	\mathbb{Z}_2	\mathbb{Z}_2	\mathbb{Z}	0	0	0
	(Hel)		\mathbf{C}	\mathcal{R}_5	0	$2\mathbb{Z}$	0	\mathbb{Z}_2	\mathbb{Z}_2	\mathbb{Z}	0	0
	$\sum_{n=1}^{\infty} T \rightarrow \overline{X} \uparrow^{\Lambda_2} $		CI	\mathcal{R}_6	0	0	$2\mathbb{Z}$	0	\mathbb{Z}_2	\mathbb{Z}_2	\mathbb{Z}	0
	$\leq 1 - \overline{\Lambda}$	U^+_{-+}, U^{+-}	BDI, CII	\mathcal{C}_1	0	\mathbb{Z}	0	\mathbb{Z}	0	\mathbb{Z}	0	\mathbb{Z}
		U_{+-}^+, U_{-+}^-	DIII, CI	C_1	0	Z	0	Z	0	Z	0	Z
	Wavevector											

222 class

Question

• Is it possible to realize essentially new structure of surface states?



Glide symmetry gives rise to distinct topological states

Mobius twist in surface states

Shiozaki-MS-Gomi(15)

glide = mirror reflection + non-primitive lattice translation



Nonsymmorphic Symmetry

Glide symmetry gives essentially new structures in topological table



[Shiozaki-MS-Gomi (15)]

$$G(k_x)\mathcal{H}(k_x,k_y,k_z)G^{-1}(k_x) = \mathcal{H}(k_x,k_y,-k_z), \ G^2(k_x) = e^{-ik_x}$$

Like topological crystalline insulators, $k_z=0$ plane can be separated into two glide subsectors



But, there is an important difference

Key point

Eigenvalues of glide operator do not have 2π periodicity in k_x



As a result, these two subsectors are connected with a twist



Correspondingly, a surface state also should have a Mobius twist structure when $k_z=0$,



Along the k_x direction, chiral edge state in $G(k\downarrow x) = e\uparrow ik\downarrow x/2$ sector is smoothly connected to anti-chiral one in $G(k\downarrow x) = -e\uparrow ik\downarrow x/2$ sector.

In addition, from the Mobius twist structure, the two glide subsectors can be exchanged adiabatically



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Interestingly, the surface state with Mobius twist can be open in the $k_{\rm x}\mbox{-direction}$



Surface state is detached from the bulk state at k_z=0 This feature can be used to identify this phase by ARPES experiments

$$G(k_x)\mathcal{H}(k_x,k_y,k_z)G^{-1}(k_x) = \mathcal{H}(k_x,k_y,-k_z), \quad G^2(k_x) = e^{-ik_x}$$
$$T\mathcal{H}(k)T^{-1} = \mathcal{H}(-k)$$

In the presence of TRS, the Kramers degeneracy at the zone boundary requires two helical modes to have the open structure.



Two chiral mode (N=2) = Two anti-chiral mode (N=-2) Z₄ topological phase



Material realization

Material realizations were quickly proposed after our finding

Hourglass fermion



- Mobius Kondo Insulator
 - CeNiSn Po-Yao Chang et al, arXiv:1603.03435



We can expect other candidates ..

Heavy fermion SCs

Summary

- Space group as well as time-reversal and particle-hole (=charge conjugation) symmetries give novel topological phases.
- Using the Hamiltonian mapping shifting symmetry, a systematic classification of TCIs and TCSCs can be done
- The nonsymmorphic symmetry provides an interesting Mobius twist structure of the surface state.